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M.C.Nemes

and

A.F.R. de Toledo Piza

UNIVERSIDADE DE SÃO PAULO
INSTITUTO DE FÍSICA
Caixa Postal - 20.516
Cidade Universitária
São Paulo - BRASIL

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M. C. NEMES*

Division de Physique Thèorique, Institut de Physique Nucléaire,
F-91406 - Orsay Cédex, France

A. F. R. de Toledo Piza

Instituto de Física, Universidade de São Paulo, C.Postal 20.516,
01000 - São Paulo, S.P., Brasil

ABSTRACT

We present a formal derivation of the exact dynamics of the one body density matrix. Its essential ingredients are shown to be: a) a mean field unitary time evolution; b) irreducible non-unitary corrections to the unitary evolution (collision effects); and c) effects due to the time evolution of initial state correlations (which contribute to both (a) and (b)). A qualitative discussion of the importance of collision effects for the expectation values of one body operators, and a quantitative illustration in the framework of an exactly soluble model are given. In this case one finds non unitary contributions as large as 100%.

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I. INTRODUCTION

The dynamical evolution of a finite, isolated, many body system is currently given as a unitary time development of a state vector or, more generally, of some state representative such as a density matrix. In a variety of different contexts, however, far simpler descriptions in terms of one body (mean field) unitary time developments have met considerable success. They include the familiar TDHF as well as mean field approximations derived by functional integral methods. In the case of TDHF, in particular, one works with simplified (determinantal) state representatives and believes their possible shortcomings to be adjusted to the simplified dynamics in such a way as to produce sensible results for some few body observables, at least.

In general one body observables are fully determined by the knowledge of the one body density associated with the state representative of the many body system. In this sense, it is governed by an open subdynamics of the overall unitary dynamics which will be, in general, non unitary itself (1). This circumstance has led to many attempts to go "beyond" the TDHF approximation. The purpose of this work is to clarify the nature of the one body subdynamics of a many fermion system, exposing clearly the origin and nature of non unitary effects and also making connections to the familiar ideas of TDHF. We show that in general the exact time evolution of the one body density matrix has non-unitary as well as unitary aspects. Non-unitary effects result from correlations dynamically produced in the many-body system and from the time development of correlations present in the initial many-body state. The unitary effects can be described in terms of a Hartree-Fock type one-body hamiltonian with unitary corrections which arise from the same sources as the non-unitary effects. A

formal derivation of the exact time-evolution of the one-body density is given in section II and discussed in section IV. In section II, we give a general discussion as the importance of non unitary effects on the time evolution of one body observables and illustrate the main points with the consideration of an exactly soluble example.

II. IMPORTANCE OF NON-UNITARY CONTRIBUTIONS TO $\frac{d\langle A\rangle}{dt}$: AN EXAMPLE

Consider the expectation value one body observables A in a time dependent context. (These are the standard objects for which TDHF has been extensively used as an approximation in the context of nuclear physics). They are fully determined by the one body density matrix of the observed system (which we choose for convenience to represent in terms of natural one body orbitals)

$$\rho_{\lambda\lambda'} = Tr\left(c^{+}_{\lambda'} c_{\lambda} F\right) = p_{\lambda}\delta_{\lambda\lambda'} \qquad \text{(II-1)}$$

where F describes the state of the system. The usual TDHF approximation is based on a determinantal ansatz for $\rho_{\alpha\beta}$ at all times. This implies a non-linear, one body (mean field) evolution of single particle states with constant unit occupation. This gives:

$$i\frac{d\langle A\rangle}{dt} = \sum_{\lambda\ occ.} \langle\lambda|[A, h_{HF}]|\lambda\rangle \qquad \text{(II-2)}$$

It should be stressed that the determinantal ansatz of the TDHF approach involves a twofold aggression to the true description of the time-evolving system. First, it implies in general the replacement of the true (in general correlated) initial

state by an uncorrelated approximation; second, it replaces the complete dynamical evolution by a unitary (mean field) one body approximation (with an appropriately chosen effective interaction in the context of nuclear structure). The importance of this twofold approximation has been recently stressed by Alhassid and Koonin (3). As mentioned in the introduction, the successes of TDHF can be seen as resulting from a happy destructive interference between these two simplifications, which is in fact nothing but a reestament of the commonly held view that the TDHF state should rather be used as a device to evaluate few body observables.

Let us leave aside, for the moment, the question of the specification of the initial state and consider more closely the properties of the exact time development of the one body density. On general grounds (1) one must have corrections not only to the unitary one body time displacement generator h_{HF}, but also non unitary effects which manifest themselves as time dependent occupation numbers p_{λ} in the one body density. Thus eq. (II-2) should be replaced by

$$i\frac{d\langle A\rangle}{dt} = \sum_{\lambda} p_{\lambda}\langle\lambda|[A, h]|\lambda\rangle + i\sum_{\lambda}\dot{p}_{\lambda}\langle\lambda|A|\lambda\rangle \qquad \text{(II-3)}$$

Note that there is no restriction in the one body character of h, but that in general h need not be of the Hartree-Fock form. Conservation of probability gives, moreover,

$$\sum_{\lambda}\dot{p}_{\lambda} = 0 \qquad \text{(II-4)}$$

This shows that the importance of the last term in eq. (II-3) will be related to the dispersion in λ of the natural orbital expectation values $\langle\lambda|A|\lambda\rangle$. Whenever these expectation values

are strongly clustered around a common value the Hartree-Fock form, eq. (II-2), displays a correct structure, as non unitary contributions to $\frac{d<A>}{dt}$ become small. This shows that an improvement of the TDHF description of the time evolution of one body densities should involve, in particular, non-unitary corrections (usually known as "collision terms"). There have been recently several versions proposed for such corrections (2), based on diverse approximations. In section III bellow, such non-unitary effects are formally isolated in an exact way. Before that, however, we exhibit the action of non-unitary effects in the context of a soluble model. It is worth stressing again that this example should be understood in the sense that the correlation free initial conditions to be used completely describe the initial state. The effect of inital state correlations will of course, be crucial in general, and will be dealt with in sections III and IV.

A simple, closed example of non unitary effects on the expectations value of a one body operator is the time dependence of $<J_z>$ (the "inversion") in the Lipkin model (9)

$$H = J_z + \frac{1}{2} tg 2\chi (J_+^2 + J_-^2) \qquad J_z = \frac{1}{2}\sum_{p\sigma} \sigma a^+_{p\sigma} a_{p\sigma} \qquad J_\pm = \sum_p a^+_{p\pm} a_{p\mp} \qquad \sigma = \pm 1 \tag{II-5}$$

In the simplest case of two particles, the exact, time dependent one body density associated with unperturbed (χ=0) ground state as initial condition is given by

$$\rho_{1+1+} = \rho_{2+2+} = 2 \sin^2\chi \cos^2\chi (1 - \cos 2\omega t)$$
$$\rho_{1-1-} = \rho_{2-2-} = \cos^4\chi + \sin^4\chi + 2\sin^2\chi\cos^2\chi \cos 2\omega t$$
$$\rho_{\alpha\beta} = 0, \quad \alpha \neq \beta \tag{II-6}$$

where $\hbar\omega = (\cos 2\chi)^{-1}$

This gives

$$<J_z>(t) = -\left[\cos^2 2\chi + \sin^2 2\chi \cos 2\omega t\right] \tag{II-7}$$

The fact that $\rho(t)$, eq. (II-6), is diagonal at all times implies time independent natural orbitals. All the time dependence appearing in eq. (II-7) comes thus from non unitary effects (namely, the time dependence of the diagonal elements - the occupations p_λ - of eq. (II-6)).

The unperturbed ground state, on the other hand, is a static solution of the Hartree-Fock approximation, stable for $\chi < \pi/8$. This means of course that the TDHF version of $<J_z>$ is time independent:

$$<J_z>_{HF}(t) = -\frac{1}{2} \tag{II-8}$$

The exact time dependence of the "inversion", eq. (II-7), together with its Hartree-Fock counter part is shown in fig. 1 for some values of χ. In this example, therefore, the difference between $<J_z>(+)$ and $<J_z>_{HF}(+)$ comes from the time dependence of the occupations p_λ and can become quite large for values of the couplong above $tg2\chi \cong .3$. Moreover these two objects are qualitatively different in terms of their time dependence. Note that the natural orbital expectation values are in this case $\pm 1/2$. As mentioned before this is an essential ingredient for the importance of non-unitary contribution to $\frac{d}{dt}<J_z>$. In fact, it is easy to verify that

$$\langle \hat{N} \rangle = 2 = \langle \hat{N} \rangle_{HF} \qquad \text{(II-9)}$$

where $\hat{N}$ is the number operator for the Lipkin model, which has degenerate natural orbital expectation values, $\langle \lambda | \hat{N} | \lambda \rangle$.

Due to the well known "parity" symmetry of the Lipkin model, the exact one body density associated with the time evolution of the unperturbed ground state of the N particle Lipkin model remains diagonal at all times. Large discrepancies between $\langle J_z \rangle$ and $\langle J_z \rangle_{HF}$ will thus occur also in the N-particle case for sufficently strong interaction term in H .

It is also interesting to consider a case where the initial condition is <u>not</u> a static solution of the Hartree-Fock approximation. We thus consider initially a determinant which, in particular, is "deformed" in the sense that it is not an eigenstate of the exact constant of motion $\hat{J}^2$:

$$|\psi(0)\rangle = c^{+}_{2+}\, c^{+}_{1+}\, |\,\rangle \qquad \text{(II-10)}$$

where the rotated single particle states $c^{+}_{p\sigma}$ $(p = 1, 2;\ \sigma = \pm)$ are defined as:

$$\begin{bmatrix} c^{+}_{p+} \\ c^{+}_{p-} \end{bmatrix} = \begin{bmatrix} e^{i\psi_p} \sin\alpha_p & \cos\alpha_p \\ \cos\alpha_p & -e^{-i\psi_p} \sin\alpha_p \end{bmatrix} \begin{bmatrix} a^{+}_{p+} \\ a^{+}_{p-} \end{bmatrix} \qquad \text{(II-11)}$$

The values of $\langle J_z \rangle(t)$ for the exact time evolution and as obtained in the TDHF approximation are plotted in Fig. 2, for the given values of α_p and ψ_p . In both cases one gets periodic results, but the periods are unrelated. Moreover, the numerical (10) TDHF solution is not harmonic while the exact values of $\langle J_z \rangle(t)$

are given by the simple closed expression

$$\langle J_z \rangle(t) = .2551 + .6228 \cos 2\omega t + .02704 \sin 2\omega t \qquad \text{(II-12)}$$

In this case both the exact occupation probabilities <u>and</u> the natural state orbitals are time dependent. A formal study of such time dependences, including the consideration of initial correlations, is given in the following section.

III. FORMAL CLOSED EQUATIONS FOR THE EXACT EVOLUTION OF THE ONE BODY DENSITY

We will here consider the question of the time evolution of the one body density matrix

$$\rho_{\alpha\beta}(t) = \langle \psi(t) | a^{+}_{\beta} a_{\alpha} | \psi(t) \rangle \qquad \text{(III-1)}$$

given the exact development of the many body state vector

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle \qquad \text{(III-2)}$$

We look for closed equations which separate explicitly unitary and non-unitary effects in the time evolution of $\rho_{\alpha\beta}(t)$. As shown in ref. (1) the unique separation of these two types of time evolution is easily achieved by using the natural orbital representation for $\rho_{\alpha\beta}(+)$.

$$\rho_{\alpha\beta}(t) \longrightarrow \rho_{\lambda\lambda'}(t) = \langle \psi(t) | c^{+}_{\lambda'} c_{\lambda} | \psi(t) \rangle = \rho_{\lambda} \delta_{\lambda\lambda'} \qquad \text{(III-3)}$$

Note that this is a time dependent representation, i.e.,

$$c^{+}_{\lambda} = c^{+}_{\lambda}(t) .$$

The real occupation probabilities p_λ are of course also time dependent in general. The (hermitean) one body generator of the unitary time evolution is defined by

$$i\dot{c}^{+}_{\lambda} = [h(t), c^{+}_{\lambda}] \qquad \text{(III-4)}$$

or equivalently, using the natural orbital representation for $h(t)$

$$i\dot{c}^{+}_{\lambda} = \sum_{\lambda'} h_{\lambda\lambda'}(t)\, c^{+}_{\lambda'} \qquad \text{(III-5)}$$

Taking the time derivative of eq. (III-3), using (III-2) and (III-5) one easily gets

$$h_{\lambda\lambda'}(p_\lambda - p_{\lambda'}) = \langle\psi(t)|[H, c^{+}_{\lambda'}c_\lambda]|\psi(t)\rangle \qquad (\lambda \neq \lambda') \qquad \text{(III-6a)}$$

$$\dot{p}_\lambda = i\langle\psi(t)|[H, c^{+}_{\lambda}c_\lambda]|\psi(t)\rangle \qquad \text{(III-6b)}$$

which identify unitary and non unitary time displacements. Note that, since we work in the natural orbital representation, the diagonal elements $h_{\lambda\lambda}$ are left undefined by eq. (III-6a). This point is discussed in more detail in Appendix A.

These are not, however, closed equations, as they involve the many body state vector $|\psi(t)\rangle$. Actually, this enters only through the expectation value of a two body operator (assuming that H has a two body character) so that what is really needed for eqs. (III-6) in addition to the one body density is the

two body density correlation function (cumulant)

$$\sigma_{\mu\nu\lambda\rho} = \rho^{(2)}_{\mu\nu\lambda\rho} - \left[\rho_{\mu\rho}\rho_{\nu\lambda} - \rho_{\mu\lambda}\rho_{\nu\rho}\right] \qquad \text{(III-7)}$$

where $\rho^{(2)}$ is the full two body density associated with $|\psi(t)\rangle$. As is well known, an attempt to get an equation for $\rho^{(2)}$ will bring in the three body density $\rho^{(3)}$ etc.. Using eqs. (III-7), eqs. (III-6) can be put into the form

$$(p_{\lambda'} - p_\lambda)h_{\lambda\lambda'} = (p_{\lambda'} - p_\lambda)h^{HF}_{\lambda\lambda'} + \frac{1}{2}\sum_{\mu\nu\rho}\left(\tilde{v}_{\lambda\nu\rho\mu}\sigma_{\rho\mu\lambda'\nu} - \tilde{v}_{\mu\nu\lambda'\rho}\sigma_{\lambda\rho\mu\nu}\right) \qquad \text{(III-8a)}$$

$$\dot{p}_\lambda = \frac{-i}{2}\sum_{\mu\nu\rho}\left(\tilde{v}_{\lambda\nu\rho\mu}\sigma_{\rho\mu\lambda\nu} - \tilde{v}_{\mu\nu\lambda\rho}\sigma_{\lambda\rho\mu\nu}\right) \qquad \text{(III-8b)}$$

The Hartree-Fock hamiltonian $h^{HF}_{\lambda\lambda'}$ is given by

$$h^{HF}_{\lambda\lambda'} = t_{\lambda\lambda'} + \sum_{\mu} p_\mu \tilde{v}_{\lambda\mu\lambda'\mu} \qquad \text{(III-9)}$$

and $\tilde{v}_{\lambda\mu\rho\sigma}$ are antisymmetrized two body matrix elements in the basis of natural orbitals. "Collision term" effects are to be associated with eq. (III-8b), of course. They are related in an essential way to irreducible two body correlations as shown by the vanishing of $\dot{p}_\lambda$ together with the two density correlation function (III-7).

We now proceed to formally close eqs. (III-6) for the time evolution of the one body density. The first crucial step for this is to obtain a decomposition of the many body density $F = |\psi(t)\rangle\langle\psi(t)|$ as

$$F = F_o + F' \qquad \text{(III-10)}$$

where F_o is such that

$$Tr(c^+_\lambda c_\lambda F_o) = Tr(c^+_\lambda c_\lambda F) = \rho_{\lambda\lambda} \qquad \text{(III-11)}$$

and all density correlation functions vanish, i.e., F_o contains no irreducible two or many particle correlations*. This implies that F_o is of the form (4) (in terms of natural orbitals)

$$F_o = \prod_\lambda \left[(1-\rho_\lambda) c_\lambda c^+_\lambda + \rho_\lambda c^+_\lambda c_\lambda\right] \qquad \text{(III-12)}$$

where the ρ_λ are the occupation probabilities of the natural orbitals. An alternative form for F_o is

$$F_o = \frac{\prod_\lambda e^{-n_\lambda c^+_\lambda c_\lambda}}{Tr\left(\prod_\lambda e^{-n_\lambda c^+_\lambda c_\lambda}\right)} \qquad \text{(III-13)}$$

with $\rho_\lambda = (1 - e^{n_\lambda})^{-1}$. This form for the uncorrelated part of the many body density carries all antissimetrization properties. In particular it gives rise, in eq. (III-19a) below, to a non

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* The development given below parallels a formalism recently given by Ayik (2). In that reference, however, the form adopted for the uncorrelated part of the many body density (eq.(2.4) there) and the related operator $C_1(t)$ (eq.(2.7)) do not deem adequate to us. In fact, uncorrelated, non determinantal many body densities are necessarily of the form (III-12) below. In particular, they have a non vanishing fluctuation of particle number (5). Due to this fact, they are best written in Fock space. The complete absence of correlations for a many body density of the form written in ref. (2) holds only for pure determinantal states. On the other hand, the time dependence of the operator $C_1(t)$ must be duly taken into account in the derivation of equations (2.10) and (2.11) of reference (2).

determiantal Hartree-Fock type contribution to the generator of unitary time displacements which includes exchange effects. This is achieved at the expense of having a nonvanishing fluctuation in particle number (5). A compensating property of course results for F', since F has a definite number of particles.

The second crucial step is to express the correlation part F' of F in terms of F which is, as seen, fully determined by the one body density. This can be formally accomplished by the construction of an operator Q in Liouville space such that

$$\dot{F}' = Q\dot{F} \qquad \text{(III-14)}$$

Q can be time dependent, but it must be determined solely in terms of the information contained in the uncorrelated part F_o of the many body density. Technical details of the constructions of Q are given in Appendix B. With such an operator the Liouville equation for the full density F

$$i\dot{F} = [H, F] \equiv LF \qquad \text{(III-15)}$$

gives

$$\left(i\frac{d}{dt} - QL\right)F' = QLF_o \qquad \text{(III-16)}$$

where equation (III-10) has been used on the r.h.s. of equation (III-15).

Introducing now the Green's function

$$G(t,t') = T\exp\left(-i\int_{t'}^{t} dt''\, Q(t'')L\right) \qquad \text{(III-17)}$$

we get

$$F'(t) = G(t,0)F'(0) - i\int_0^t dt' G(t,t')Q(t')L F_0(t') \qquad \text{(III-18)}$$

which is as close as we can get to our aim. Note that an initial correlation term involving F'(0) still remains. Eq.(III-18) expresses the correlation part of the full density at time t in terms of a time integral over the past of the uncorrelated density F_0 plus initial correlation terms. This shows that the complete elimination of correlations can only be achieved when the initial state is such that F'(0)=0. This was the case, in particular, for the example discussed in the preceeding section.

Using this result, eqs. (III-6) can be written as

$$h_{\lambda\lambda'}(p_\lambda - p_{\lambda'}) = Tr\left([H, c^+_{\lambda'}c_\lambda]G(t,0)F'(0)\right) +$$
$$+ Tr\left([H, c^+_{\lambda'}c_\lambda]F_0\right) - i\,Tr\left([H, c^+_{\lambda'}c_\lambda]\int_0^t dt' G(t,t')Q(t')LF_0(t')\right) \qquad \text{(III-19a)}$$

$$\dot{p}_\lambda = i\,Tr\left([H, c^+_\lambda c_\lambda]G(t,0)F'(0)\right) +$$
$$+ Tr\left([H, c^+_\lambda c_\lambda]\int_0^t dt' G(t,t')Q(t')L F_0(t')\right) \qquad \text{(III-19b)}$$

This closes eqs.(III-6) except for initial correlation terms, which must then be supplied together with the one body initial conditions in order to determine the full time evolution of the one body density. Actually eq.(III-18) contains far more information than needed in eqs. (III-6). In fact, only the two density correlation function of F'(t) enters in eqs. (III-19) as discussed in connection with eqs. (III-8) above. The fact that the full correlation part is needed to obtain the exact time evolution of this object prevents one from dealing just with the minimally required final information at all times. The second term on the r.h.s. of eq.

(III-19c) simply reproduces the H.F. hamiltonian. The first and last terms of the same equation represent respectively initial state and dynamical unitary correlation terms which correct the mean field.

In order to bring out the crucial effects of initial state correlations for the reduced one body dynamics we may consider the particular case of the density associated with a (fully correlated) stationary state of H as initial state. In this case we must have $\dot{p}_\lambda = 0$ and $\dot{c}^+_\lambda = \varepsilon_\lambda c^+_\lambda$, i.e., constant occupation probabilities and diagonal one body unitary displacement generator $h_{\lambda\lambda'}$. This is achieved, in general, as a result of the cancelation of nondiagonal elements in the second term in the r.h.s. of eq. (III-19a) (the "Hartree-Fock-like" time displacement generator) with compensating non-diagonal terms arising from the first term, i.e., due to the two-density correlation function of the stationary initial state. At t=0 the last term in this equation obviously vanishes.

IV. DISCUSSION

There are two types of question to be considered in connection with the possible use of eqs.(III-19). On the one side one must deal with the problem of a treatable implementation of the formal objects such as G(t,t') and Q(t') which appear in these equations. On the other side, one must face the problem of initial state correlations. Due to the interplay of the later with the dynamics these two questions must be dealt with consistently. We will not attempt here to carry this program further, and limit ourselves to a brief discussion of other approaches which have been put forth to deal with these questions.

It should be noted from the very start that this approach relies on an adequate description of the state of the

system. The values of (one body) observables appear as deduced quantities. The "contraction of the description" involved in eqs. (III-19) consists in retaining the minimum essential information required to fully deal with the special class of one body observables. This approach is to be contrasted with other methods which attempt to calculate directly the values a few relevant observables, without an explicit consideration of the quantum state of the system in general. Functional integration methods associated with stationary phase approximations have been wildely used in this sense (6), (7). An alternative variational approach within this framework has recently been put forth by Balian and Veneroni (8). Here, one "contracts the description" through the device of restricting the variational spaces slowed for state representatives and observables treated in a complementary fashion. One obtains in this way dynamical equations which are in general specific to the chosen observables, so that no general validity can be attributed to the state description. While such concentration on the values of a few required observables may be of pragmatic value in that it allows for a greater technical simplification, it gives nevertheless limited insight on the general dynamical behavior of the system. As a result of this the accuracy of the obtained results is difficult to assess.

Even though eqs. (III-19) are not directly amenable to calculation, they reveal the nature of the minimum dynamical ingredients which are required for a full description of the one body aspects of a many body system. They include in general full information on the initial state correlations and the full history of the uncorrelated part of the density. This later information eventually suffices to determine correlation aspects arissing dynamically which are not directly tied to the initial state correlations. In the soluble example given in section II we considered cases which involved no initial correlations

(determinantal initial states). It should be stressed that, according to our point of view, these initial states are taken to be fa thful representatives of the state of the system rather than approximations to it. The non-unitary one body effects obtained from the exact solution can thus in principle be obtained also from the time development for $t > 0$ of the uncorrelated part of the full density alone, in this case, as shown in eq. (III-19b). If one uses instead the approach of ref. (8), restricting oneself to general uncorrelated densities (which in the case of the example can fully describe the initial state) and to one body operators, one gets a fully unitary time development. All dynamical correlation effects are thus missed. As shown in eq. (II-3) they are generally present. Their quantitative importance depends on the particular observable under consideration. In the particular case of the example, we found important quantitative effects for $\langle J_z \rangle$.

APPENDIX A

We discuss in this appendix some apparent ambiguities in the determination of the one-body unitary time displacement operator in terms of eq. (III-6a). These ambiguities stem from two facts: (a) only $\lambda \neq \lambda'$ terms are allowed in eq. (III-6a), so that diagonal elements $h_{\lambda\lambda}$ are left undefined; and (b) a bothersome zero factor appears in the l.h.s. of this equation in the case of equal one-body occupation probabilities in different natural orbitals, i.e., $p_\lambda = p_{\lambda'}$ with $\lambda \neq \lambda'$.

Concerning point (a), it sufices to note that the equation which gives the time development of the one body density in the representation of its natural orbitals $|\lambda\rangle$ (note that this is a time-dependent representation)

$$\rho = \sum_\lambda |\lambda\rangle \rho_\lambda \langle\lambda| \tag{A-1}$$

reads

$$i\frac{d\rho}{dt} = \sum_{\lambda\lambda'} \left[h_{\lambda\lambda'} |\lambda'\rangle \rho_\lambda \langle\lambda| - |\lambda\rangle \rho_\lambda \langle\lambda'| h_{\lambda'\lambda} \right] + i \sum_\lambda |\lambda\rangle \dot{\rho}_\lambda \langle\lambda| \tag{A-2}$$

Both unitary and non-unitary effects appear in this equation, and the structure of the unitary term (first on the r.h.s.) shows directly that diagonal matrix elements $h_{\lambda\lambda}$ make a vanishing contribution.

In order to deal with point (b) it is convenient to look at eq. (III-6a) rewritten in the form (III-8a):

$$\left(h_{\lambda\lambda'} - h^{HF}_{\lambda\lambda'}\right)(\rho_{\lambda'} - \rho_\lambda) = \Delta_{\lambda\lambda'} \tag{A-3}$$

where the anti-hermitean matrix $\Delta_{\lambda\lambda'}$ is given in terms of the two-body potential v and of the two-density correlation function σ as

$$\Delta_{\lambda\lambda'} = \frac{1}{2} \sum_{\mu\nu\rho} \left(\tilde{v}_{\lambda\nu\rho\mu} \sigma_{\rho\mu\lambda'\nu} - \tilde{v}_{\mu\nu\lambda'\rho} \sigma_{\lambda\rho\mu\nu} \right) \tag{A-4}$$

The freedom associated with occupation degeneracy now allows for the selection of natural orbitals which diagonalize the matrix $\Delta_{\lambda\lambda'}$ (including diagonal terms!) in the subspace of natural orbitals with degenerate occupation. This guarantees the consistency of eq. (A-3) (note that $\lambda \neq \lambda'$ there) but still leaves $h_{\lambda\lambda'}$ undefined. It is also easy to show, however that the time developement (A-2) of the one body density becomes independent of $h_{\mu\nu}$ when the orbitals μ and ν have equal occupation. In fact writing out explicitely the terms of (A-2) which involve $h_{\mu\nu}$ and $h_{\nu\mu}$ (the prime in the first sum below indicates the ommission of such terms)

$$\begin{aligned} i\frac{d\rho}{dt} = {\sum_{\lambda\lambda'}}' \left[h_{\lambda\lambda'} |\lambda'\rangle \rho_\lambda \langle\lambda| - |\lambda\rangle \rho_\lambda \langle\lambda'| h_{\lambda'\lambda} \right] + i \sum_\lambda |\lambda\rangle \dot{\rho}_\lambda \langle\lambda| + \\ + h_{\mu\nu} |\nu\rangle \rho_\mu \langle\mu| - |\mu\rangle \rho_\mu \langle\nu| h_{\nu\mu} \\ + h_{\nu\mu} |\mu\rangle \rho_\nu \langle\nu| - |\nu\rangle \rho_\nu \langle\mu| h_{\mu\nu} \end{aligned} \tag{A-5}$$

we see immediately that, when $\rho_\mu = \rho_\nu$, these terms cancel out exactly.

It should be stressed that the occupations of the degenerate orbitals still change as prescribed by $\dot{\rho}_\mu$ and $\dot{\rho}_\nu$. These are, up to a factor of i, the eigenvalues of the matrix $\Delta_{\lambda\lambda'}$ within the degenerate subspace. It is only the unitary part of the time evolution which becomes irrelevant there. This

is in fact an obvious consequence of the invariance of the one-body density under one-body unitary transformations performed within subspaces with degenerate occupation.

APPENDIX B

We describe here the construction of the operator Q appearing in eq. (II-14). It should be emphasized from the start that Q is time dependent and is not (and, in fact, need not be) a projection operator. In order to allow for the closure of eqs. (III-6) it must fulfill condition (III-14) and be fully determined by the uncorrelated part F_o of the full density F.

Consider first the sequence of operators (cf eqs. (III-12) and (III-13)) indexed by the integer N

$$P_N \bullet = \sum_{\nu=1}^{N} \Bigg[\prod_{\substack{\mu=1 \\ \mu\neq\nu}}^{N} \left\{ (1-p_\mu) c_\mu c_\mu^+ + p_\mu c_\mu^+ c_\mu \right\} \times \Big(c_\nu^+ c_\nu \, \mathrm{Tr}(c_\nu^+ c_\nu \bullet) + c_\nu c_\nu^+ \, \mathrm{Tr}(c_\nu c_\nu^+ \bullet) \Big) \Bigg] - (N-1) \prod_{\mu=1}^{N} \left\{ (1-p_\mu) c_\mu c_\mu^+ + p_\mu c_\mu^+ c_\mu \right\} \mathrm{Tr} \bullet \qquad \text{(B-1)}$$

If we let P_N act on F we clearly get a trunceted version of eq. (III-12) where the product is restricted to N terms. We may therefore write

$$F_o = \lim_{N\to\infty} P_N F \equiv P F \qquad \text{(B-2)}$$

where P is hermitean, time-dependent and is such that $P F_o = P F$ so that it acts like a projection operator when acting on F. Note however that for any other Liouville vector the idempotent property of P does not hold (note that P_N is defined by eq. (B-1) where the c-numbers p_μ and the second quantized operators c_μ^+, c_μ are defined in terms of the one body density associated with F, at time t)

Using eq. (B-2) we can now write

$$F' = (1-P)F \qquad \text{(B-3)}$$

which does not lead directly to (III-14) in view of the time dependence of P. In fact

$$\dot{F}' = (1-P)\dot{F} - \dot{P}F \qquad \text{(B-4)}$$

The last term of eq. (B-4) can be evaluated in a straightforward way as $\lim_{N\to\infty} \dot{P}_N F$. We get, using eqs. (III-5) and (III-6a) to handle time derivatives of the c^+_μ, c_μ,

$$\dot{P}F = -i \sum_\nu \sum_{\mu<\nu} \prod_{\lambda\neq\mu,\nu} \left[(1-\rho_\lambda)c_\lambda c^+_\lambda + \rho_\lambda c^+_\lambda c_\lambda\right] \times$$

$$\times \left[c^+_\mu c_\nu \, \mathrm{Tr}(c^+_\nu c_\mu L F) + c^+_\nu c_\mu \, \mathrm{Tr}(c^+_\mu c_\nu L F)\right] \qquad \text{(B-5)}$$

Since, moreover, $LF = i\dot{F}$, we can take eq. (B-5) as defining an operator $\tilde{P}$ such that

$$\dot{P}F = \tilde{P}\dot{F} \qquad \text{(B-6)}$$

Note that the ingredients which enter in the construction of $\tilde{P}$ appear already in P, eq. (B-2).

Taking this result now back into eq. (B-4) we are finally left with

$$\dot{F}' = (1-P-\tilde{P})\dot{F} \equiv Q\dot{F} \qquad \text{(B-7)}$$

which completes the construction of Q.

REFERENCES

1) M.C.Nemes and A.F.R. de Toledo Piza - Preprint IFUSP/P-287, August 1981, to be published.

2) C.Y.Wong and H.H.K.Tang - Phys.Rev.Lett. 40, 1070 (1978); H.Orland and R.Schaeffer, Zeit. fur Physik A290, 191 (1978); S.Ayik, Zeit. fur PhysikA298, 83 (1980); P.Grangé, H.A.Weidenmuler and G.Wolschin - Preprint MPI H-1981 v.8; G.Mantzouranis and H.C.Pauli - Zeit. fur Physik A281,165 (1977) and Phys.Rev. C22, 1550 (1980); R.Balian and M.Veneroni, Saclay Preprint, DPH-T/81-017.

3) Y.Alhassid and S.E.Koonin - Phys.Rev. C23, 1590 (1981).

4) P.-O.Lowdin - Phys.Rev. 97, 1474 (1955).

5) J.Des Cloizeaux - In Many Body Physics, edited by C. De Witt and R. Balian (Gordon and Breach, N.Y. 1968) pp.5-36.

6) S.Levit - Phys. Rev. C21, 1594 (1980). A.K.Kerman and S.Levit - Phys.Rev. C24, 1029 (1981) and references therein.

7) J.P.Blaisot and M.Orland - Journal de Physique Lett. 41, L-53 (1980); M.Kuratsuji and T.Suzuki - Phys.Lett. 92B, 19 (1980).

8) R. Balian and M. Veneroni - Saclay Preprint DPH-T/81-67.

9) A.Glick, H.J.Lipkin and N.Meshkov - Nucl.Phys. 62, 118,199 and 211 (1965).

10) M.Nielssen - M.Sc.Thesis, University of São Paulo, 1981 (unpublished).

FIGURE CAPTIONS

FIG. 1 - The expectation value $\langle J_z \rangle$ for the two-particle Lipkin model as a function of time. The dashed line shows exact values for the unperturbed (x=0) ground state as initial condition and several values of x. The full line at $\langle J_z \rangle = -1$ is the TDHF expectation value (stationary in this case) for the same initial condition.

FIG. 2 - The expectation value $\langle J_z \rangle$ for the two-particle Lipkin model as a function of time for the initial condition $\alpha_1=70^\circ$; $\alpha_2=85.9^\circ$; $\psi_1=45^\circ$; $\psi_2=0^\circ$ and for tg 2x=-1.5.

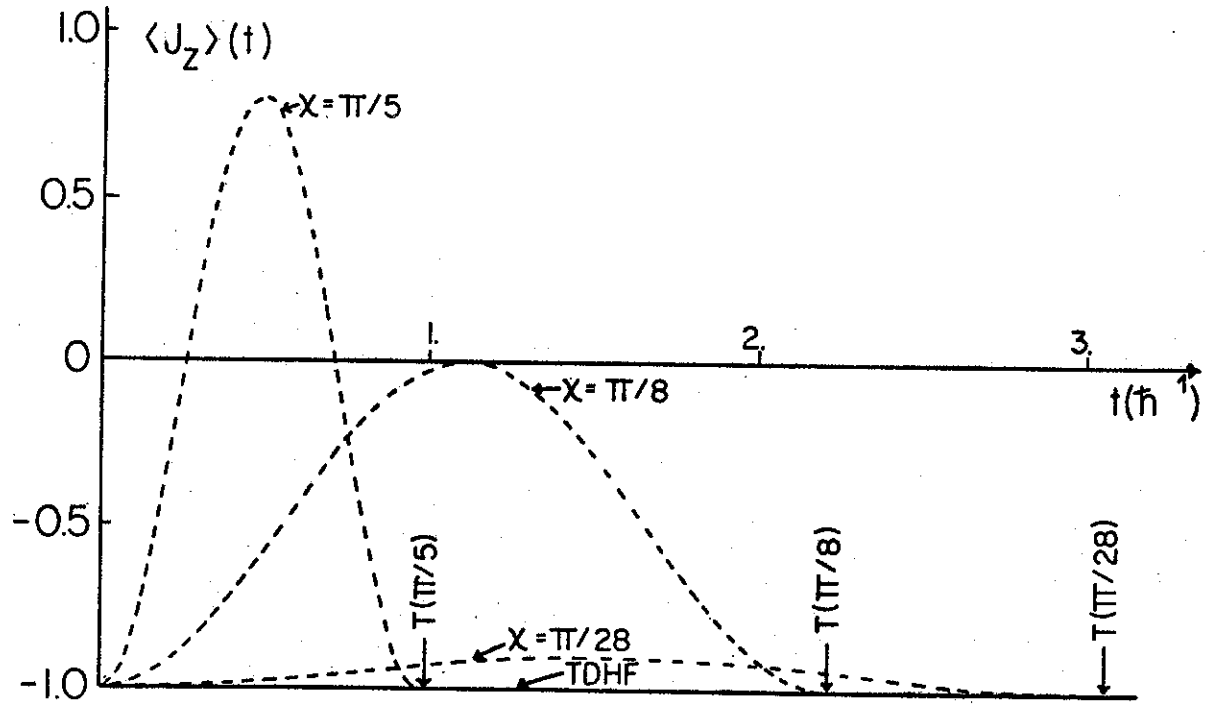

FIGURE 1

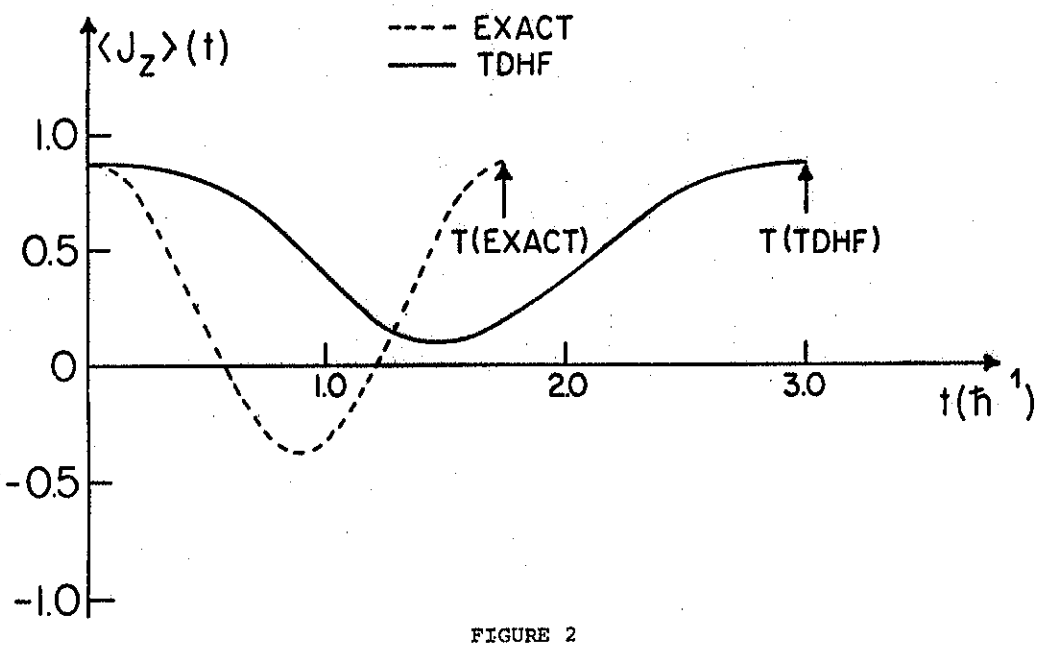

FIGURE 2