HOW COLLISION TERMS RELATE TO THE DYNAMICS OF QUANTUM CORRELATIONS*

A.F.R. de Toledo Piza
Inst. Física, USP, CP 20516, 01000 São Paulo, Brasil

1. INTRODUCTION

Time dependent, self consistent mean field theories approximate the time evolution of interacting quantum subsystems in terms of a set of effective, coupled unitary time displacement laws for the subsystems themselves. This offers the enormous simplification of avoiding the dynamic entanglement of the individual subsystems that would in general result from the complete dynamical law, due to time evolving correlations among them. It implies also, however, that the approximate state-representatives (density matrices) become inadequate at least in so far as the effects of such a dynamical entanglement are lost: the degree of quantum coherence of state-representatives of subsystems is preserved by the unitary mean field law but is in general altered by the exact evolution. Collision terms are non-unitary corrections to time dependent mean field theories which attempt at redressing this defect while still retaining as much as possible of the simplification offered by these theories. In the following development, based on refs. (1) and (2), I will describe a way of scrutinizing the works of the exact dynamical law so as to isolate unitary (mean field) and non-unitary (collision) effects in the effective time-displacement laws for subsystems. This will also throw some light on the general connection between non-unitary effects and the dynamics of intersubsystem correlations. After that, I will indicate how one can proceed in order to obtain a description of effective dynamical laws for subsystems, including both unitary and non-unitary effects, which is as much as possible closed in terms of the disentangled state-representatives themselves, and finally comment on possible further reductions of the theory aimed at making it fit for consumption.

2. COLLECTIVE/INTRINSIC SUBSYSTEMS

Even though I will eventually turn to nuclear one-body mean fields, it is easier to begin with the consideration of two sub-systems as in the case of some damped collective mode of a nuclear system. Here the subsystems are characterized respectively in terms of distinct (commuting) collective (typically few, symmetric) and intrinsic (typically many) degrees of freedom; and the Hilbert space for the system

may be naturally considered as a product of a collective and an intrinsic space:

$$H = H_C \otimes H_I \ .$$

The quantum state of the composite system will be described by a normalized vector $|\psi>$ of this product space, or alternatively by a projection operator of trace one, $F = |\psi><\psi|$. (This implies that I am adopting a restriction to pure quantum states of the composite system. While it is possible to work with more general states, this simplifies the discussion and illustrates all the relevant points). Furthermore, given the state F, one can obtain the corresponding state-representatives for each of the two subsystems by taking partial traces of this object. Thus

$$\rho = Tr_I F \qquad \text{and} \qquad R = Tr_C F$$

are the appropriate subsystem state representatives in H_C and in H_I respectively. These are hermitean operators of trace one, but they are not in general projectors, which means that the subsystem states are in general not pure states, but mixtures. Choosing the representations which diagonalize these operators, one can write them as

$$(1) \quad \rho = \sum_k |c_k>p_k<c_k| \qquad \text{and} \qquad (2) \quad R = \sum_k |I_k>p_k<I_k|$$

where the $|c_k>$ and the $|I_k>$ are orthornormal "natural states", defined as the eigenvectors of ρ and R respectively. The fact that these operators have the same spectrum is a result of the theory of Hilbert-Schmidt kernels, as shown in detail by von Neumann[3]. Associated with it is the existence of a priviledged decomposition of the state vector $|\psi>$ as

$$(3) \quad |\psi> = \sum_k \alpha_k |c_k> \otimes |I_k> \qquad \text{with} \qquad p_k = \alpha_k^2 \ .$$

The common eigenvalues p_k reveal, therefore, the degree of entanglement of the two subsystems in the state $|\psi>$: one single nonvanishing eigenvalue implies uncorrelated subsystems (factored state $|\psi>$), while the existence of a large number of nonvanishing eigenvalues implies strongly intercorrelated subsystems.

I will now state how dynamics appears in terms of this representation. As F evolves in time in accordance with the Liouville-von Neumann equation

$$(4) \qquad i\dot{F} = [H,F] \equiv LF$$

where H is the Hamiltonian of the composite system, both the natural states, $|c_k\rangle$ and $|I_k\rangle$, and the eigenvalues p_k will also evolve in time. Since at any time the natural states constitute orthonormal sets, their time evolution can be described in terms of hermitean time-displacement generators $h^{(c)}(t)$ and $h^{(I)}(t)$ respectively. Thus, in particular

$$i \frac{d}{dt} \left[|c_k\rangle\langle c_k| \right] = \left[h^{(c)}(t), |c_k\rangle\langle c_k| \right]$$

which allows one to write the time derivative of eq. (1) as

$$(5) \qquad i\dot{\rho} = \sum_{k\ell} |c_k\rangle (p_\ell - p_k)\, h^{(c)}_{k\ell} \langle c_\ell| + i \sum_k |c_k\rangle \dot{p}_k \langle c_k| \quad .$$

Here $h^{(c)}_{k\ell} \equiv \langle c_k|h^{(c)}|c_\ell\rangle$. A similar form results of course for the time-derivative of eq. (2), involving $h^{(I)}$ and states $|I_k\rangle$. By inserting (3) into eq. (4) one can moreover deduce algebraically that

$$(6) \qquad (p_\ell - p_k) h^{(c)}_{k\ell} = \alpha_\ell \langle c_k I_\ell|H|\psi\rangle - \langle\psi|H|c_\ell I_k\rangle \alpha_k \qquad (k \neq \ell)$$

$$(7) \qquad (p_\ell - p_k) h^{(I)}_{k\ell} = \alpha_\ell \langle c_\ell I_k|H|\psi\rangle - \langle\psi|H|c_k I_\ell\rangle \alpha_k \qquad (k \neq \ell)$$

and $$(8) \qquad \dot{\alpha}_k = \mathrm{Im} \langle c_k I_k|H|\psi\rangle \quad ,$$

relating the dynamical ingredients of eq. (5) to the complete dynamics of the composite system.

The effective dynamics of the subsystem described by ρ (the "collective" subsystem) is clearly splitt into two parts of diverse nature in eq. (5). The first part comes from the time evolution of the natural states and is fully unitary. Let me call this the "mean field" part. It is governed by the effective generator $h^{(c)}$. This, in the special correlation free case in which $F = \rho R$ (i.e., the state vector $|\psi\rangle$ is a simple product state), reduces just to $\mathrm{Tr}_I HR$, but otherwise is more complicated: the mean field part will depend, in general, on correlation effects. The second part involves time rates of change of eigenvalues of the hermitean ρ, and is thus essentially non unitary. Let me call it the "collision" part. Its form, taken in conjunction with eqs. (8) and (3), shows that it arises out of the time evolution of the degree of entanglement of the subsystems, this being characterized by the set of weights entering into the priviledged expansion (3).

It will have been noticed that the basic trick allowing for the separation of a unitary "mean field" part from a non-unitary,"collision" part on the r.h.s. of eq. (5) resides in the use made of the natural states. Thus, except for the all-important "external" ingredient consisting in the adopted initial factorization of the Hilbert space H (i.e., the "a priori" characterization of each of the two subsystems), it is an "intrinsic" trick, in the sense that it operates in terms of properties of the state vector itself, rather than of properties depending on some base in which it may find itself expanded. This trick is quite general, and has in fact been used as such in the work of Wong and Tang on collision terms[4] but occurs also in a work of 1935 by Schrödinger[5].

Next for consideration is the fact that eq. (5), together with the corresponding equation for $\dot{R}$, are not closed equations. Their essential dynamical ingredients involve again all the information present in the fully correlated, time dependent state $|\psi>$ through eqs.(6), (7) and (8), so that the question concerning the possibility of effectively closing them in terms of ρ and R arises naturally. This can be acomplished by writing the density F as $F = \rho R + F'$ and then eliminating formally the traceless correlation part F' after substituting this form in eq. (4). In this way one can replace eq. (5) by[1,6]

$$(9)\quad i\dot{\rho}(t) = \mathrm{Tr}_I\left[L(t,0)F'(0)\right] + \mathrm{Tr}_I\left[LR(t)\right]\rho(t) - i\int_0^t dt'\,\mathrm{Tr}_I\left[K(t,t')R(t')\rho(t')\right]$$

and a similar equation for $\dot{R}(t)$. The Liouvillian memory kernel $K(t,t')$ describes the buildup of correlations out of the uncorrelated part ρR of F; and the first term on the r.h.s. describes the effects at time t of the existing correlations at time zero, $F'(0)$. Thus, to the extent that these effects make themselves felt at time t, one cannot eliminate completely the information contained in the correlation part F' of F.

Rather than elaborate on the content of this type of equation and of its ingredients in the present context, I will now swich to the consideration of a one-body subdynamics of a many-body system. The question of closing the description will then lead to contact with one-body mean field theories and "Time-Dependent Hartree-Fock collision terms".

3. ONE-BODY SUBSYSTEM

Switching to the case of the one-body subdynamics is actually

straightforward, implying a deep structural afinity between the treatment of collective and single nucleon subsystems from the present point of view. The important differences that will eventually emerge will all hinge on physical rather than structural properties of the two types of subsystem. One may, in fact, directly take ρ of eq. (1) to be the one-body density associated with the fully correlated A-body state $|\psi>$. At the same time, R becomes the corresponding (A-1)-body density, while eqs. (5)-(8) translate the dynamical law, eq. (4), into this language. Eq. (3) also exists in this case. Adopting an explicit configuration space representation it becomes, in fact

$$(10) \qquad <x_1 \ldots x_A|\psi> = \sum_k \alpha_k <x_1|c_k><x_2 \ldots x_A|I_k> \quad .$$

It should be observed that Pauli correlations are treated in eq. (10) on the same footing with all other correlations: if $|\psi>$ is a determinantal state, eq. (10) reduces to a row expansion of the appropriate normalized determinant of rank A. Moreover, in eqs. (5)-(8) the product states are not antisymmetrized, but the appropriate projection results automatically from the antisymmetry of $|\psi>$ and from the symmetry of H. It is actually easy to check that eqs. (6) and (8) can be rewritten in second quantized form as

$$(11) \qquad (p_\ell - p_k) h^{(c)}_{k\ell} = \frac{1}{A} <\psi| \left[c^+_\ell c_k, H \right] |\psi> \qquad (k \neq \ell)$$

and

$$(12) \qquad i \dot{p}_k = \frac{1}{A} <\psi| \left[c^+_k c_k, H \right] |\psi> \quad ,$$

where the fermion creation operators $c^+_k(t)$ are associated with the one-body natural orbitals $|c_k>$ of eq. (1), and $\sum_k p_k(t) = 1$. The reduced one-body subdynamics associated with eq. (4) appears thus in the guise of eq. (5), the two terms on its r.h.s. giving respectively the mean field part and the collision part of an effective one-body Liouvillian. These objects are determined by eqs. (6) and (8), or by eqs. (11) and (12), in terms of the complete information contained in the fully correlated state $|\psi>$.

It is of course possible to carry the paralelism of the present one-body case with the collective/intrinsic case further and obtain a pair of formal coupled equations for ρ and R by eliminating a traceless correlation part F' defined as before by $F = \rho R + F'$. This sin-

gles out a given particle and treats Pauli and dynamical correlations on the same level, a somewhat unphysical option which may be particularly ill-suited for approximate treatments. It is in fact preferable in this case to give a privileged status to Pauli correlations and to treat all particles in a symmetric fashion. This is accomplished by defining a different traceless correlation part $F_1^!$ of the full density through $F = F_0 + F_1^!$ where F_0 is best written in Fock space as[7]

$$F_0 = \prod_k \left[(1-Ap_k)\, c_k c_k^+ + Ap_k\, c_k^+ c_k \right] \quad . \tag{13}$$

The formal elimination of the correlation part $F_1^!$ can be carried out essentially as in the collective/intrinsic case yielding for eqs. (11) and (12) respectively

$$(p_\ell - p_k) h_{k\ell}^{(c)} = \frac{1}{A} \mathrm{Tr}\left[c_\ell^+ c_k L_1(t,0) F_1^!(0) \right] + \frac{1}{A} \mathrm{Tr}\left[c_\ell^+ c_k \left(L F_0(t) - i \int_0^t dt' K_1(t,t') F_0(t') \right) \right] , \quad k \neq \ell \tag{14}$$

and

$$i \dot{p}_k = \frac{1}{A} \mathrm{Tr}\left[c_k^+ c_k L_1(t,0) F_1^!(0) \right] - \frac{i}{A} \mathrm{Tr}\left[c_k^+ c_k \int_0^t dt' K_1(t,t') F_0(t') \right] \quad . \tag{15}$$

As was the case with eq. (9), these expressions carry memory effects involving both the "uncorrelated" density F_0 and initial correlations $F_1^!(0)$. The cooresponding memory kernels ar given by

$$K_1(t,t') = LG(t,t')Q(t')L \quad \text{and} \quad L_1(t,0) = LG(t,0) \tag{16, 17}$$

where

$$G(t,t') = T\exp\left(-i \int_{t'}^{t} d\tau\, Q(\tau) L\right) \tag{18}$$

and $Q(t)$ is a Liouville operator with the property $\dot{F}_1^! = Q\dot{F}$. It can be constructed entirely out of ingredients occuring in F_0, namely the occupation probabilities $p_k(t)$ and the associated states $c_k^+(t)$, and is given explicitely in ref. (2). I will refrain from giving more details here, and just state that what it does essentially is to select only relevant many-particle correlation parts from the objects upon which it acts.

4. DISCUSSION: ONE-BODY MEAN FIELD AND COLLISION EFFECTS

Together with eq. (5), eqs. (14) and (15) perform the decomposition of the effective one body subdynamics into unitary and non-unitary parts in as closed a form as possible. The big breach is again the unavoidable involvement of the initial correlations $F_1^!(0)$ in both parts. The term involving LF_0 in eq. (14) gives rise to a unitary contribution of standard Hartree-Fock form, involving the one body density ρ of eq. (1). A corresponding term is absent from eq. (15). Finally, terms involving K_1 represent contributions due to dynamically generated many-body correlations.

Before any further commitment on the significance or use of these equations it is crucial to recall what are the physical facts standing behind them in the context of nuclear dynamics: in few words, single-particle, mean field approximations to nuclear dynamics only became successfull and respectable when carried considerably beyond the limits of a straight Hartree-Fock context. Because of radical properties of nucleon-nucleon forces, adequate success required the consideradion of effective, density dependent interactions designed so as to account for the effects of essential correlations induced by these forces. It must certainly be considered a remarkable fact that it has been possible to include enough correlations via the effective forces with completely coherent (determinantal) one body densities in a closed theory for such densities in the static case[8]. Extentions to dynamical situations ("Time-Dependent Hartree-Fock") involve certainly a good deal of extrapolation of the more carefully controlable applications to nuclear ground states, but quantitative successes are still impressive.

In such a framework, the correlation dependent terms of eq. (14) acquire a special significance if one intends to keep some connection to more fundamental levels of description. In fact, at least part of the correlation effects become essential ingredients to produce a sufficiently healthy effective mean field: it is now well known that the bare LF_0 term of eq. (14) is not good enough for that. Actually, current TDHF calculations with effective forces should rather be interpreted in terms of the replacement of the full r.h.s. of that equation by the effective Hartree-Fock field under the assumption of a determinantal one body density and frozen one body occupation probabilities, $\dot{p}_k = 0$, instead of eq. (15). This implies of course a truncation "by ansatz" of all non-unitary effects and furthermore restricts in principle dynamical correlation corrections to the mean field by forcing

them through the gauge of the effective two body interaction.

The collision part of the effective dynamical law as given by eq. (15), on the other hand, can be seen to depend in an essential way on objects which are rigorously the "diagonal" (i.e., $k = \ell$) counterparts of the correlation corrections to the time-dependent effective mean field part, eq. (14) (cf. also eqs. (11) and (12)). These are however just the corrections to the mean field which can at best be described as being obtained, in the dynamical case, by extrapolation of results obtained in stationary contexts. It is clear moreover that the "diagonal" contributions of eq. (15) must vanish in the stationary case. Present knowledge of these objects is therefore extremely meager.

Even so, and in order to have an exploratory idea of the possible content of eq. (15), one may look into the structure of the second term on the r.h.s. of eq. (15) assuming that, as in the case of the mean field part, the remaining initial correlation term has been sufficiently taken into account in terms of a suitable effective interaction in the memory kernel K_1, eq. (16). The relevant object is then

$$\mathrm{Tr}\; c_k^+ c_k \int_0^t dt' \Big[H, G(t,t')Q(t')\big[H, F_0(t')\big]\Big]$$

from which, under customary weak-coupling|Markof approximations[9,10] one can readily obtain a Boltzmann-like collision term including the appropriate occupation factors which account for the exclusion principle. It looks thus as this form constitutes a stable structural element, at least in the weak-coupling limit, in the sense that it does not appear to be sensitive to the meanders of particular derivations[9-11]. Details are however overshadowed by the uncertainties in the effective interactions.

I cannot sufficiently acknowledge two rather short periods of intense work in São Paulo and complementary periods of stimulating correspondence with M.C. Nemes. As the references indicate, this was crucial for the elaboration of this report.

REFERENCES

* Work supported in part by CNPq and FAPESP (Brasil)
1) M.C. Nemes and A.F.R. de Toledo Piza, Preprint IFUSP/P-287, August 1981

2) M.C. Nemes and A.F.R. de Toledo Piza, Preprint IFUSP/P-317, February 1982
3) J. von Neumann, Mathematical Foundations of Quantum Mechanics, Princeton U. Press 1955, chap. VI
4) C.Y. Wong and H.H.K. Tang, Phys. Rev. Lett. 40, 1070 (1978)
5) E. Schrödinger, Proc. Camb. Phil. Soc. 31, 555 (1935); ibid. 32, 446 (1936). See also O. Kübler and H.D. Zeh, Ann. Phys. (N.Y.) 76, 405 (1973)
6) C.R. Willis and R.H. Picard, Phys. Rev. A9, 1343 (1974)
7) J. Des Cloiseaux, in Many Body Physics, C. De Witt and R. Balian, eds., Gordon and Breach, N.Y. 1968, pp. 5-36.
8) J.W. Negele, MIT Preprint CTP#898, October 1981 (to be published in Revs. Mod. Phys.)
9) P. Grangē, H.A. Weidenmüller and G. Wolschin, Preprint MPIH-1981 v.8, to be published in Ann. Phys. (N.Y.) (and references therein)
10) S. Ayik, Zeit. für Physik A298, 83 (1980); Preprint GSI-81-12 (May 1981).
11) H.C. Pauli, Heidelberg preprint MPI H-1982-V7.