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OF COLLISION TERMS

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ABSTRACT

Collision terms are non-unitary corrections usually added to mean field descriptions in order to describe dissipative effects. Derivations of collision terms usually include assumptions which lack an explicit connection with a fully quantum dynamical description. We examine the quantum dynamical foundations of collision terms: they are shown to reflect the dynamics of quantum correlations. A careful study of the non-unitary aspects of the evolution of quantum correlations leads naturally to an unambiguous definition of a collision term. This collision term is shown to obey a non-linear pre-master equation, whose derivation is fully quantum-mechanical. Moreover, we show that quantum correlations also yield a unitary correction to the mean field description, which could be absorbed in a suitable redefinition of the mean field. Formal expressions for these corrections are derived and their connection with memory effects exhibited explicitly. The typical time of evolution of quantum correlations allows for an analytical expression for the "lifetime of mean field descriptions". Finally, a quantum mechanical point of view for "irreversibility" in deep inelastic is discussed.

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0. INTRODUCTION

Besides being useful in many other areas of Physics, mean field theories are expected to provide good approximations to many important aspects of nuclear dynamics. However, the description of heavy ion collisions in terms of such theories is not entirely satisfactory: the measured dispersion of observables like the final mass and energy distributions cannot be correctly reproduced. In this context, an important program consists in obtaining corrections to the mean field dynamics.

The basic structure of a mean field theory typically involves a working decomposition of the physical system under consideration (e.g. many body nuclear system) in a number of subsystems described in terms of independent (commuting) dynamical variables. Decompositions frequently used, and of recognized utility, include the distinction between "collective" and "intrinsic" degrees of freedom (a decomposition involving two subsystems) and the consideration of the constituent nucleons themselves as subsystems. The main point is then to replace the actual interaction between subsystems by a suitably defined average interaction in order to avoid their hopeless entanglement through the works of the complete dynamical law. Ion-ion interactions given in terms of just a few collective variables and Hartree Fock fields are well known examples of such replacement interactions.

This simplification, however, can only be made at the cost of renouncing the sufficiently accurate description of all but a restricted set of dynamical variables associated with the adopted subsystems (e.g. one body operators in TDHF). Moreover, the truncated part of the interaction between subsystems may lead to serious inaccuracies even for predictions concerning the dynamical variables of this restricted set. A possible way to avoid this last difficulty is to devise corrections to the mean

field dynamics in order to incorporate to it at least part of the effects that would be due to the entanglement of the subsystems without having to deal explicitly with it. These are the corrections usually known as "collision terms". Several approaches to the collision corrections to TDHF exist now in the literature^(1,2,3,4,5), and a number of treatments of the effects of the coupling of the scattering degrees of freedom to the "intrinsic" dynamics of heavy ions can also be considered from this point of view.

Derivations of collision terms usually include assumptions which lack an explicit connection to a fully quantum dynamical description of the process under consideration. In particular, dissipative effects are introduced by these collision terms which, in principle, would seem alien to quantum mechanics, a time reversal invariant theory⁽⁶⁾. It is the aim of this paper to examine the quantum dynamical foundations of the collision terms: they will be shown to reflect the dynamics of quantum correlations. In fact, collision corrections can be regarded as a redressing, at the level of particular subsystems, of quantum correlation effects washed out by the averaging process inherent to the mean field approximation. On quite general grounds, we show that these effects are of two different types: a) intersystem correlations will affect the nature of the generator of unitary time translations of the subsystems and b) the development in time of the correlations which will give non-unitary corrections to the time development of the state of the subsystems. To the extent that a unitary evolution of the subsystems under consideration is taken to characterize the mean field time development, it follows that the corrections of type b) constitute the "irreducible collision effects". The formal identification of these effects with the dynamics of quantum correlations leads to an unambiguous definition of collision terms as corrections to mean field theories.

On the other hand, corrections of type a) even though also originating from quantum correlations, can be incorporated in a suitable redefinition of the mean fields themselves. In particular, these effects will not change the quantum coherence properties of the subsystems, unlike the corrections of type b).

Moreover, a formal identification of the "irreducible collisions effects" will allow us to define the "lifetime of a mean field description" as being the characteristic time of evolution of quantum correlations, and to give a quantitative measure for it.

In section I, we present the formalism we use to study quantum correlations and apply it to derive mean field approximations. The Hartree-Fock hamiltonian is obtained as an example and the evolution of quantum correlations for short times (and minimally correlated initial states) is shown to be characterized by a non unitary bistochastic matrix. The characteristic time of this evolution is taken as the "lifetime of the mean field description". In section II we show that the dynamics of quantum correlations have two distinct effects on the mean field description. These effects are discussed and formal expressions for them are derived. In particular, the non unitary aspects of the evolution of quantum correlations is shown to be associated with the "irreducible collision effects" and to obey a pre-master equation, whose derivation is exact and fully quantum dynamical. A quantum mechanical point of view for the "irreversible" aspects in Deep Inelastic Collisions is then discussed and in section III we use it to analyse the dissipative aspects of two different theoretical approaches to Deep Inelastic, namely, the statistical theory of Agassi et al. (7) and the Coherent Surface Model of Broglia et al. (8). We close with a brief discussion.

I. A FORMALISM TO STUDY QUANTUM CORRELATIONS

A natural framework to study the dynamics of quantum correlations is a decomposition of quantum states used by Schrödinger in 1935⁽⁹⁾ to analyse the interrelations of interacting quantum subsystems. It allows in particular for a clear distinction between effects a) and b) above. The detailed properties of the various ingredients appearing as a result of the decomposition hinge crucially on the choice of subsystems. Thus the detailed behavior of all correlation effects and of "irreducible collision effects" in particular appear as subsystem specific. They reflect no more than the consequences of the unitary evolution of the full system for the effective evolution of a restricted set of selected observables.

We shall present here the Schrödinger decomposition and analyse its properties for pure states. The extension for mixtures involves a straightforward reformulation in Liouville space and is given in Appendix A.

I-A. THE FORMALISM (KINEMATICS)

Any vector $|\psi\rangle$ contained in the tensor product of two Hilbert spaces $\mathcal{H} = \mathcal{H}_C \otimes \mathcal{H}_I$ can be expanded in the Schmidt canonical form⁽¹⁰⁾

$$|\psi\rangle = \sum_i \alpha_i |c_i\rangle |I_i\rangle \quad (\text{I-1})$$

where $\{|c_i\rangle\}$ and $\{|I_i\rangle\}$ are certain orthonormal systems in \mathcal{H}_C and \mathcal{H}_I , respectively. These systems may always be completed to form basis systems. The basis systems are uniquely defined by the state $|\psi\rangle$ except for degeneracy of the coefficients α_i . This includes in particular the degeneracy of all basis states

used to complete the basis, i.e., those affected with a vanishing coefficient α_i in (I-1). From this expansion one readily obtains the density matrices of the two subsystems in diagonal form as

$$\rho = \text{tr}_I |\psi\rangle\langle\psi| = \sum_i |c_i\rangle\langle c_i| \alpha_i^2 \quad (\text{I-2})$$

$$\rho_c = \text{tr}_c |\psi\rangle\langle\psi| = \sum_i |I_i\rangle\langle I_i| \alpha_i^2 \quad (\text{I-3})$$

The information about subsystem c(I) is contained in $\rho(R)$. The density matrices ρ and R are generally von Neuman mixtures, which are seen to be thus conveniently represented in terms of their orthonormal "natural states" $\{|c_i\rangle\}$ and $\{|I_i\rangle\}$ respectively. These are always discrete sets for states $|\psi\rangle$ of finite norm (this is a consequence of Hilbert-Schmidt theorem⁽¹¹⁾, noting that R and ρ are trace class hermitian operators in \mathcal{H}_I and in \mathcal{H}_c respectively).

The following properties of this decomposition should be emphasized:

- a) the spectra of R and ρ are the same.
- b) From the normalization condition of the state $|\psi\rangle$, $\langle\psi|\psi\rangle = 1$, it follows that

$$\sum_i \alpha_i^2 = 1$$

c) The decomposition is unique for a given choice of subsystems, (i.e., for a given factorization of the Hilbert space as $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_I$), except for the usual ambiguities relative to eigenvalue degeneracy.

d) From (I-2) and (I-3) an entropy can be defined for the subsystems as

$$\begin{aligned} S_c &= -\text{tr}_c \rho \ln \rho = S_I = -\text{tr}_I R \ln R = -\sum_i \alpha_i^2 \ln \alpha_i^2 \equiv \\ &\equiv -\sum_i p_i \ln p_i \quad (p_i = \alpha_i^2) \end{aligned} \quad (\text{I-4})$$

e) The coefficients $\alpha_i(p_i)$ describe correlations between the two subsystems. It can be seen from (I-1) that the number of coefficients α_i which are different from zero gives the minimum number of terms of a decomposition of $|\psi\rangle$ in terms of factorized basis states.

I-B. THE DYNAMICS

The Schrödinger representation (I-1) defines also a decomposition of the quantum dynamics of the composite system.⁽¹²⁾ First, due to the orthonormality at all times of the states $|c_i\rangle$ and $|I_i\rangle$, their time evolution can be written as

$$i \frac{d}{dt} |c_i(t)\rangle = h_c(t) |c_i(t)\rangle \quad (\text{I-5})$$

$$i \frac{d}{dt} |I_i(t)\rangle = h_I(t) |I_i(t)\rangle \quad (\text{I-6})$$

where h_c and h_I are hermitean, in general time dependent time-diplacement generators.

The time dependent amplitudes $\alpha_i(t)$ can be taken to be real with no loss of generality and from

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle = \sum_i \alpha_i(t) |c_i(t)\rangle |I_i(t)\rangle \quad (\text{I-7})$$

one gets the following equations which sufficiently determine h_c and h_I and give the time evolution of the amplitudes $\alpha_i(t)$

(special situations in case of degeneracy still allow a sufficient determination of these quantities - see Appendix B)

$$(\alpha_i \pm \alpha_k) (\langle I_k | h_I | I_i \rangle \pm \langle c_i | h_c | c_k \rangle) = \\ = \langle I_k c_i | H | \psi \rangle \pm \langle \psi | H | I_i c_k \rangle \quad (i \neq k) \quad (I-8)$$

$$\alpha_k (\langle c_k | h_c | c_k \rangle + \langle I_k | h_I | I_k \rangle) = \text{Re} \langle c_k I_k | H | \psi \rangle \quad (I-9)$$

$$\dot{\alpha}_k = \text{Im} \langle c_k I_k | H | \psi \rangle \quad (I-10)$$

The last equation implies probability conservation

$$\frac{d}{dt} \sum_i p_i = 0 \quad (I-11)$$

Due to the fact that this basis is time and initial state dependent it is hard to work with. However, it is ideal to study the dynamics of quantum correlations because of two important properties:

a) it displays the minimal form of correlation between subsystems (decomposition into minimum number of product states) and maximal coherence of each subsystem considered separately ($|c_i\rangle$ and $|I_i\rangle$) and their associated quantum fluctuations, together with respective statistical weight p_i .

b) It separates clearly time displacement generators associated to each subsystem from the time evolution of correlations. Note that, from eq. (I-10), it is easy to check that the time evolution of correlations implies non unitary time evolution of the reduced density matrices R and ρ . It is therefore the best candidate to be associated with collision terms.

I.C. MEAN FIELD APPROXIMATIONS

In this framework, mean field theories are obtained from the unitary time development of natural states with fixed (by constraint) occupation. Formally they can be derived if we eliminate, by constraint, the time dependence of the coefficients α_i , i.e., let

$$\dot{\alpha}_k = 0$$

instead of eq. (I-10). This, together with eq. (I-8) and (I-9) can be used to obtain sufficient information about the hermitian generators. If there are no correlations in the initial state, the usual mean field theories appear. In general, initial state correlations can be included and "generalized mean field approximation" obtained which include corrections due to the assumed initial correlation.

These statements are best illustrated by means of two examples.

Let us first take the case with no initial correlations, i.e.,

$$|\psi(0)\rangle = |c_0\rangle |I_0\rangle \quad (I-12)$$

This implies $\alpha_0 = 1$, $\alpha_{i \neq 0} = 0$ and those values will be held fixed for all times. The resulting time development of the state $|c_0\rangle$ is given by

$$i \frac{d}{dt} |c_0\rangle = \sum_{i=0}^{\infty} |c_i\rangle \langle c_i | h_c | c_0 \rangle \quad (I-13)$$

where the necessary matrix elements of h_c can be obtained from (I-8) and (I-9).

$$\langle c_0 | h_c | c_i \rangle = \langle c_0 I_0 | H | c_i I_0 \rangle = \langle c_0 | \langle H \rangle_I | c_i \rangle \quad (\text{I-14})$$

hence

$$i \frac{d}{dt} |c_0\rangle = \sum_{i=0}^{\infty} |c_i\rangle \langle c_i | \langle H \rangle_I | c_0 \rangle \quad (\text{I-15})$$

Analogously

$$i \frac{d}{dt} |I_0\rangle = \sum_{i=0}^{\infty} |I_i\rangle \langle I_i | \langle H \rangle_c | I_0 \rangle \quad (\text{I-16})$$

Note an ambiguity in the separate determination of $\langle c_0 | h_c | c_0 \rangle$ and $\langle I_0 | h_I | I_0 \rangle$. This reflects an irrelevant phase ambiguity of the factor states in the product $|c_0 I_0\rangle$.

Obviously, the mean field approximation obtained in this way (i.e., by imposing the condition $\dot{\alpha}_k = 0$) will be sustainable as a good approximation as long as the correlation effects would not be important anyway. Characteristic time associated with the evolution of the $\alpha_k(t)$ will thus determine the "lifetime of the mean field description". This time can be estimated in the following way: for short times after $t=0$,

$$\begin{aligned} \alpha_i &\approx \dot{\alpha}_i(0) t \\ \alpha_0^2 &\approx 1 - t^2 / \tau^2 \end{aligned} \quad (\text{I-17})$$

where $\tau^2 = \left(\sum_i \dot{\alpha}_i^2(0) \right)^{-1}$ from the conservation of probability. Thus, the change of the correlations for short time intervals will be characterized by the characteristic time τ given by

$$\tau^2 = \left[\sum_{k \neq 0} \langle c_0 I_0 | H | c_k I_k \rangle \langle c_k I_k | H | c_0 I_0 \rangle \right]^{-1} \quad (\text{I-18})$$

Note that, from (I-9), $\langle c_k I_k | H | c_0 I_0 \rangle$ is pure imaginary for $k \neq 0$. Furthermore, according to (I-8), unoccupied states are to be chosen such that

$$\langle c_i I_j | H | c_0 I_0 \rangle = 0, \quad i \neq j, \quad i, j \neq 0 \quad (\text{I-19})$$

The time τ can then be evaluated as

$$\tau^2 = \left[\langle c_0 I_0 | H (1 - |c_0\rangle \langle c_0|) (1 - |I_0\rangle \langle I_0|) H | c_0 I_0 \rangle \right]^{-1} \quad (\text{I-20})$$

This of course just means that the transitions from $|c_0 I_0\rangle$ which change correlations are those that feed the doorway $|D\rangle$,

$$|D\rangle = N (1 - |c_0\rangle \langle c_0|) (1 - |I_0\rangle \langle I_0|) H | c_0 I_0 \rangle \quad (\text{I-21})$$

$$\text{Thus } \tau^2 = |\langle c_0 I_0 | H | D \rangle|^{-2}$$

In eq. (I-21) N is a normalization factor. The form of $|D\rangle$ contains a restriction on all transitions changing the initial state consisting in the exclusion of those which do not change its factorized form (I-12).

This shows moreover that, for short times, the evolution of the occupation probabilities $p_i(t) = \alpha_i^2(t)$ can be written as

$$p_i(t) = \sum_j M_{ij}(t) p_j(0) \quad (\text{I-22})$$

with $\{p_i(0)\} = \{1, 0, 0, \dots\}$ and

$$M_{ij}(t) = \begin{cases} 1 - t^2 \sum_{k \neq 0} | \langle c_k \bar{I}_k | H | c_j \bar{I}_j \rangle |^2 & i=j \\ t^2 | \langle c_i \bar{I}_i | H | c_j \bar{I}_j \rangle |^2 & i \neq j \end{cases} \quad (I-23)$$

Thus, for small but finite t , $M_{ij}(t)$ is a non unitary bistochastic matrix. Consequently the mixing character of the probability distribution $\{p_i(t)\}$ increases, a characteristic feature of many irreversible processes¹³. In particular, this implies that

$$S_c [p_i(t)] > S_c [p_i(0)] \quad (I-24)$$

As a second example, we consider a Slater determinant as the initial state, i.e.,

$$|\psi(0)\rangle = \frac{1}{\sqrt{A!}} \text{Det} [u_i(\vec{r}_j)]_{i,j=1, \dots, A} \quad (I-25)$$

and write the decomposition which singles out the coordinate \vec{r}_1 :

$$|\psi(0)\rangle = \sum_{k=1}^A \frac{1}{\sqrt{A}} u_k(\vec{r}_1) \frac{(-1)^{k+1}}{\sqrt{(A-1)!}} \text{Det} [u_i(\vec{r}_j)]_{\substack{j=2, \dots, A \\ i \neq k}} = \sum_{k=1}^A \alpha_k |c_k \bar{I}_k\rangle \quad (I-26)$$

Here we have $\alpha_k = \frac{1}{\sqrt{A}}$, $k=1, \dots, A$, which describes the Pauli correlations*. For a general hamiltonian containing one and two body terms

(*) This degeneracy, however, is not to be handled with the technique given in Appendix B. This is due to the fact that the Fermi statistics restricts the state of the system to lie in the antisymmetric sector of the space generated by $|c_i \bar{I}_j\rangle$, $i, j \leq A$. In the present case this is a one-dimensional subspace (i.e., it reduces to $|\psi(0)\rangle$). Note that the decomposition (I-26) does not automatically preserve antisymmetry (i.e., for general coefficients α_k).

$$H = \sum_e t_e + \frac{1}{2} \sum_{m \neq l} v_{ml} \quad (I-27)$$

the generator h_c is given by

$$\langle c_j | h_c | c_k \rangle = \langle c_j | t | c_k \rangle + \sum_{\substack{i \neq k \\ i \in A}} \langle c_j c_i | v | c_k c_i - c_i c_k \rangle \quad (I-28)$$

which is just the Hartree-Fock hamiltonian. As done in the previous example, one can also evaluate the lifetime of this mean field description as

$$\tau^2 = |\langle \psi(0) | H | D \rangle|^{-2} \quad (I-29)$$

where now the doorway $|D\rangle$ is given as

$$|D\rangle = N A [1 - P_c] [1 - P_I] H |\psi(0)\rangle \quad (I-30)$$

with

$$P_c = \sum_{i=1}^A |c_i\rangle \langle c_i| \quad (I-31)$$

and

$$P_I = \sum_{i=1}^A |I_i\rangle \langle I_i| \quad (I-32)$$

It can be verified that $|D\rangle$ contains two particle two-hole excitation of $|\psi(0)\rangle$ and that this result is the same found by Griffin⁽¹⁴⁾ from a different analysis.

Explicitly

$$\tau^2 = (\tau_c)^2 \frac{1}{A} \sum_{\substack{i,j \leq A \\ k,l \in A}} | \langle c_i c_j | v | c_k c_l - c_l c_k \rangle |^2$$

If we now study the short-time evolution of the probability distribution associated with the correlations displayed in eq. (I-26), we find that again it can be cast in the form of a

bistochastic matrix which is non-unitary for $t \neq 0$.

Finally a general comment on the implications of the value of the characteristic time τ is in order. As it is clear from the discussion, this time is associated with the time rate of change of the correlations as a result of the full quantum mechanical time evolution of the system, for a given prepared state. This state is thereby assumed to correspond to a full description of the system at $t=0$. To the extent that the restricted set of observables that one considers may be insensitive to the correlations generated by the full dynamical law (such a restriction being in a way implied by the adopted factorization of the phase space in the first place, e.g. one body operators in the Hartree Fock example), the limitation indicated by a given value of τ may be even grossly overpessimistic. In other words, while correlation corrections to the mean field evolution of a prepared state will evolve in a time of order τ , the quantitative predictions of the mean field theory for the appropriate observables may be reliable for longer times. A time limit to the reliability of mean field predictions would be set rather by the time it takes for the collision effects to change appreciably the state of the subsystem with respect to the pure mean field prediction. This depends on the relative quantitative importance of non unitary versus unitary ingredients of the time evolution of the subsystem.

II. THE TWO DISTINCT CORRELATION CORRECTIONS TO THE MEAN FIELD DESCRIPTION

The dynamics of quantum correlations will introduce two different types of corrections to the mean field approximation, as discussed in the introduction. The first one will be a modification of the mean field hamiltonian, and will not change the

unitary nature of the time evolution. The second one contains the "irreducible collision effects" and introduces non unitary corrections to the mean field evolution. In this section we prove these statements and also derive expressions for the two corrections.

In order to do this, it is of interest to obtain expressions for the time evolution of ρ and R where the correlations do not appear explicitly. This can be accomplished in a standard way, using the projection technique described in (15) at the expense of introducing suitable memory effects. The technique we use to single out the two different corrections is the following: First we write the memory terms in the representation introduced in the previous section, because in that representation the separation between unitary time evolution of subsystems densities and non-unitary collision terms is natural and unambiguous. This shows clearly that the effects of correlations, as contained in the memory term are of the two distinct types mentioned above and yields closed expressions for them.

We begin by writing the full density F (which for simplicity we assume to be associated with a pure quantum state $|\psi\rangle$) as

$$F = |\psi\rangle\langle\psi| = R\rho + F' \quad (\text{II-1})$$

where R and ρ are defined as before (eq. (I-2) and (I-3)).

Using the methods of reference (15) we obtain the coupled equations for the densities as

$$i\dot{\rho} = \tau_I (L'F'(0)) + L_C \rho + \langle L' \rangle_{I,t} \rho - i \int_0^t \langle \Delta_t L' G(t,t') \Delta_{t'} L' \rangle_{I,t'} \rho(t') dt'$$

$$i\dot{R} = \tau_C (L'F'(0)) + L_I R + \langle L' \rangle_{C,t} R - i \int_0^t \langle \Delta_t L' G(t,t') \Delta_{t'} L' \rangle_{C,t'} R(t') dt' \quad (\text{II-2})$$

Here we used $H = H_C + H_I + H'$ and a corresponding separation of the liouvillian L . Brackets denote averaging over the appropriate densities at times indicated in the subscript. We defined

$$\Delta_t L' = L' - \langle L' \rangle_{I,t} - \langle L' \rangle_{c,t} \quad (\text{II-3})$$

and used

$$G(t,t') = T \exp \left(-i \int_{t'}^t dt'' [1 - P(t'')] L \right) \quad (\text{II-4})$$

where

$$P(t) = R(t) \tau_c + \rho(t) \tau_I - R(t) \rho(t) \tau_c \tau_I \quad (\text{II-5})$$

$P(t)$ is a time dependent projection operator. It has the property

$$P(t) F = R \rho. \quad (\text{II-6})$$

The first term on the r.h.s. of the coupled equations comes from initial correlations, i.e., F' at $t=0$. At this time the memory terms obviously vanish. We may immediately notice, moreover, that at any time t , the memory terms may be replaced by correlation terms as

$$-i \int_0^t \langle \Delta_t L' G(t,t') \Delta_{t'} L' \rangle_{I,t'} \rho(t') dt' = \tau_I (L' F'(t)) \quad (\text{II-7})$$

provided one has $F'(0)=0$, namely, in the absence of initial correlations. From here on we restrict ourselves to this case.

The contribution from the memory term, eq. (II-7)

contains all correlation effects. Using the Schrödinger decomposition of $|\psi\rangle$ and the definitions of F' (eq. (II-1)) we get,

$$L' F'(t) = \left[H', \sum_{ijkl} |c_i I_j\rangle \langle \alpha_i \alpha_k \delta_{ij} \delta_{kl} - \alpha_i^2 \alpha_j^2 \delta_{ik} \delta_{jl} \rangle \langle c_k I_l | \right] \quad (\text{II-8})$$

from which we obtain in a straightforward way

$$\tau_I (L' F'(t)) = -\langle L' \rangle_{I,t} \rho + [h_c - H_c, \rho] + i \sum_j |c_j\rangle \dot{p}_j \langle c_j| \quad (\text{II-9a})$$

or, equivalently,

$$\tau_I (L' F'(t)) \equiv \tilde{L}_{\text{corr}} \rho + i \sum_j |c_j\rangle \dot{p}_j \langle c_j| \quad (\text{II-9b})$$

The first term on the right hand side of (II-9a) gives the required correction to the unitary evolution of ρ . It has vanishing diagonal elements in the representation of natural states $|c_i\rangle$:

$$\tilde{L}_{\text{corr}} \rho = \sum_{i,j \neq i} |c_i\rangle \Delta p_{ij} \langle c_j| \quad (\text{II-10})$$

The last term is the "irreducible collision term" which, as explicitly shown, is fully diagonal in this representation. We may thus write, using (II-7)

$$\Delta p_{\ell m} = -i \langle c_\ell | \int_0^t \langle \Delta_t L' G(t,t') \Delta_{t'} L' \rangle_{I,t'} \rho(t') dt' | c_m \rangle \quad (\text{II-11})$$

($\ell \neq m$)

and also

$$\dot{p}_i = \langle c_i | \int_0^t \langle \Delta_t L' G(t,t') \Delta_{t'} L' \rangle_{I,t'} \rho(t') | c_i \rangle \quad (\text{II-12})$$

Analogous expressions hold for the corresponding objects in the equation for R. The characteristic features of corrections (II-11) and (II-12) can be made more conspicuous if we express the bracketed part of the integrand in terms of natural states at the appropriate times as

$$\langle \Delta_{t'}^L G(t, t') \Delta_{t'}^{L'} \rangle_{T, t'} = \sum_{j, j', e, e'} |c_j(t) c_{e'}(t)\rangle \sum_{i, i'} \Gamma_{j i l i'; j' k j k'}(t, t') p_i(t') (c_{j'}(t') c_{e'}(t')) \quad (II-13)$$

The round bra-kets on the r.h.s. are a Liouville space notation for the Hilbert space operators $|c_j\rangle \langle c_{e'}|$ and $|c_{j'}\rangle \langle c_{e'}|$ respectively. Inserting this notation in eq.(II-11) we get

$$\Delta_{l m}^p = -i \int_0^t dt' \sum_{i j k} \Gamma_{i l m'; j k j k'}(t, t') p_j(t') p_k(t') \quad (l \neq m) \quad (II-14)$$

This correction involves past probabilities in the characteristic non linear fashion of self consistent mean field theories. It has vanishing diagonal matrix elements in the natural representation for time t.

We now proceed to obtain a closed equation for the probabilities $p_i(t)$ from eq. (II-12). Inserting (II-13) in (II-12) we get,

$$\dot{p}_e = \int_0^t dt' \sum_{i j k} \Gamma_{i l i l'; j k j k'}(t, t') p_j(t') p_k(t') \quad (II-15)$$

Conservation of probability $\sum_e \dot{p}_e = 0$, allows us to bring this equation to the form of a non linear pre-master equation

$$\dot{p}_e = \int_0^t dt' \sum_{i, j, k} \Gamma_{i l i l'; j k j k'}(t, t') p_j(t') p_k(t') - \int_0^t dt' \sum_{i, j, k} \Gamma_{i k i k'; j l j l'}(t, t') p_j(t') p_l(t') \quad (II-16)$$

This form is of course exact. Independently of the explicit introduction of random ingredients, it can exhibit "irreversible behavior"⁽⁶⁾. This will of course depend on the dynamics. As an example it is enough to consider a situation in which a markovian approximation makes sense: the dynamics should be such that the time dependence of $p(t')$ is slow in comparison with the time cut-off contained in $\Gamma(t, t')$. This will lead to a non linear master equation, possibly with time dependent transition probabilities.

It is interesting to notice that the appearance of "irreversible behavior" will depend crucially on two factors: a) the global dynamics; b) the particular subsystem chosen. It might be that a different choice of subsystems would NOT exhibit "irreversibility", even if the global dynamics is the same. This means, in other words, that from the point of view of quantum correlations, different sets of subsystems exhibit different aspects of the dynamics.

III. DEEP INELASTIC AND CORRELATIONS

In order to apply eqs. (II-2) to deep inelastic processes between heavy nuclei we may take the reduced density ρ to describe the collective degrees of freedom involved in the relative motion of fragments, while other, intrinsic variables are carried by R. As $t \rightarrow \infty$ we have separated out going fragments,

a situation which implies the vanishing of the interaction terms H' (or L'). In this situation all information, such as relative momentum, and orbital angular momentum, regarding the state of relative motion of the fragments can be retrieved from ρ alone. Moreover, energy conservation allows one to deduce from this information a corresponding energy distribution for the intrinsic subsystem. An adequate treatment of the correlation between collective and intrinsic subsystems is of course essential for one to be able to establish such a correspondence⁽⁶⁾. The knowledge of ρ is thus what is required to obtain the information relevant for objects like $d^2\sigma/d\Omega dE$.

However, eqs. (II-2) express the time evolution of the reduced densities ρ and R in terms of a pair of coupled equations. The equation containing R , in particular, involves again all the complications of the nuclear many body problem. Any program aiming at a calculation of ρ must therefore include a procedure enabling one to effectively deal with these complications.

The Coherent Surface Excitation Model (CSM) of Broglia, Dasso and Winther^(8,16,17) can be readily understood as providing one such simplifying procedure. Schematically, this model attempts at an extreme simplification of the intrinsic dynamics by means of a judicious choice of a few simple relevant degrees of freedom to be treated explicitly, namely the surface vibration modes of the colliding fragments. Furthermore a classical limit to the full quantum dynamics implied in eqs. (II-2) is taken. Thus, starting from the full quantum Liouville-von Neuman equation for the density F (eq. (II-1))

$$\dot{F} = \frac{1}{i\hbar} [H, F] \quad (\text{III-1})$$

we can write to lowest order in \hbar

$$\dot{F}_\omega = \{ H_\omega, F_\omega \} \quad (\text{III-2})$$

where the curly bracket denotes now a Poisson bracket of the Weyl transform H_ω of H and the Wigner transform F_ω of F ⁽¹⁸⁾.

This linear, first order partial differential equation for the full Wigner transform F_ω contains eqs. (II-2) under the stated assumptions. By making a decomposition of F_ω analogous to eq. (II-1) we can in fact derive coupled equations which are formally identical to eqs. (II-2) using appropriately defined projection operators⁽¹⁵⁾. Alternatively, we may just note that eq. (III-2) is nothing but the classical Liouville equation for phase space distributions of the system under consideration. Its characteristics are just classical trajectories for H_ω . Thus, the information which would be obtained from a solution of the coupled equations analogous to eqs. (II-2) is also given by a direct solution of eq. (III-2), which can in turn be reduced to finding the classical trajectories of H_ω . This will also include, in particular, the effects of all correlations which survive the classical approximation used for the coupled dynamics.

We turn now to a discussion of initial conditions. For sharply defined classical initial conditions, i.e.,

$$F_\omega(\vec{P}, \vec{a}, \vec{\pi}, \vec{\xi}; t=0) = \delta(\vec{P}-\vec{P}_0) \delta(\vec{a}-\vec{a}_0) \delta(\vec{\pi}-\vec{\pi}_0) \delta(\vec{\xi}-\vec{\xi}_0) \quad (\text{III-3})$$

where \vec{P} and \vec{Q} refer to collective, $\vec{\xi}$ and $\vec{\pi}$ to intrinsic degrees of freedom, it follows from eq. (II-2) that

$$F_\omega(\vec{P}, \vec{a}, \vec{\pi}, \vec{\xi}; t) = \delta(\vec{P}-\vec{P}(t)) \delta(\vec{a}-\vec{a}(t)) \delta(\vec{\pi}-\vec{\pi}(t)) \delta(\vec{\xi}-\vec{\xi}(t)) \quad (\text{III-4})$$

where $\vec{P}(t=0) = \vec{P}_0$, etc. are a classical trajectory of H_ω .

This shows explicitly that in this case the correlation part of F_w , F_w' , vanishes identically and thus that there are no correlations developing in time and no memory effects in a description analogous to eqs. (II-2). It was found in refs. (8), (16) and (17), however, that effects due to quantum fluctuations of the initial intrinsic states are of importance. These can be included in a straightforward way by replacing the sharp initial conditions for $\vec{\xi}$ and $\vec{\pi}$ by the Wigner transform f_w of the appropriate initial quantum state. One has then to consider solutions of eq. (III-2) subject to the initial condition

$$F_w(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}; t=0) = \delta(\vec{P}-\vec{P}_0) \delta(\vec{Q}-\vec{Q}_0) f_w(\vec{\pi}, \vec{\xi}) \quad (\text{III-5})$$

Writing now the initial conditions for a classical trajectory of H_w in terms of positions and momenta at time t ,

$$\begin{aligned} \vec{Q}(0) &= \vec{Q}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t) \\ \vec{P}(0) &= \vec{P}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t) \\ \vec{\xi}(0) &= \vec{\xi}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t) \\ \vec{\pi}(0) &= \vec{\pi}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t) \end{aligned}$$

we have ⁽¹⁹⁾

$$\begin{aligned} F_w(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}; t) &= \delta(\vec{P}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t) - \vec{P}_0) \delta(\vec{Q}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t) - \vec{Q}_0) \\ &\times f_w(\vec{\pi}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t), \vec{\xi}_0(\vec{P}, \vec{Q}, \vec{\pi}, \vec{\xi}, t)) \end{aligned} \quad (\text{III-7})$$

which now includes correlation effects involving \vec{P} , \vec{Q} and the

intrinsic degrees of freedom. To the extent that the distribution f_w is introduced as an essential artifact of quantum mechanics, these correlations can be described as a quantum mechanical effect. Note that they embody the conservation of energy along classical trajectories, so that the time evolution given by eq. (III-7) goes beyond just the average energy conservation typically given by mean field theories.

A possible alternate way of dealing with the difficulties of the many body problem in the second eq. (II-2) involves an attempt at effectively decoupling the two equations by means of a suitable set of consistent statistical assumptions on the interaction H' (or L') and on the reduced density R . We do not pursue this further here. We note however that a connection should be possible between the resulting effective equation for ρ and eq. (6.4) of ref. (7) in view of the fact that they give the same asymptotic information. Such a connection would be especially interesting as it would provide a link between the statistical approach of ref. (7) and the CSM.

IV. DISCUSSION

In the preceding sections we described a quantum mechanical scheme in which the characterization of collision corrections to mean field theories is unambiguous and complete. From the point of view developed there "irreversibility" effects are not alien to the full quantum evolution law, provided one considers observations done on a specified subsystem of the entire quantum system. A consequence of this is that such effects can be subsystem specific. They just reflect the entanglement of the observed subsystem and the remainder of the entire system through the works of the complete dynamical evolution.

This scheme could moreover provide for a natural framework in which to study possible connections between different attitudes regarding the treatment of the many degrees of freedom involved in a process like the deep inelastic collisions between heavy ions. Thus, while the CSM attempts at the utmost simplification of the intrinsic dynamics to be treated explicitly, statistical approaches can be seen as an attempt of taking advantage of the high complexity of the same intrinsic subsystem. It might conceivably be expected that both attitudes can eventually be made to converge in that they give reasonable descriptions of the loss of coherence of a particular subsystem which results from the dynamics of quantum correlations.

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APPENDIX A

SCHRÖDINGER DECOMPOSITION IN LIOUVILLE SPACE

The density matrix F describing the mixed state of a quantum system can be realized as a vector in Liouville space, i.e., the direct product of the Hilbert space of state vectors with its dual space. Whenever the state vector space is in turn realized as the direct product of two different spaces (implying the decomposition of the physical system into two subsystems), a corresponding factorization can be immediately extended to the Liouville space.

Let $\{|a_i\rangle \otimes |b_j\rangle\}$ be a factorized base in the Hilbert space of state vectors. The corresponding factorized base in Liouville space is written as

$$\{|A_\alpha\rangle \otimes |B_\beta\rangle\}; \alpha \equiv (i, j); \beta \equiv (k, l)$$

where the correspondence between Liouville space (round) bra-kets and state vector bra-kets is taken to be

$$|A_\alpha\rangle \longleftrightarrow |a_i\rangle \langle a_j|$$

$$|B_\beta\rangle \longleftrightarrow |b_k\rangle \langle b_l|$$

We can thus write any density F as

$$F = \sum_{\alpha\beta} f_{\alpha\beta} |A_\alpha\rangle \otimes |B_\beta\rangle$$

The analogue of the Schrödinger representation of an ordinary state vector $|\psi\rangle$ (v. eq. (I-1)) can now be obtained

by diagonalizing the hermitean matrix

$$M_{\alpha\gamma} = \sum_{\beta} f_{\alpha\beta} f_{\gamma\beta}^*$$

Thus, using the unitary transformation $\{U_{\alpha\beta}\}$ such that

$$\sum_{\beta\gamma} U_{\alpha\beta}^+ M_{\beta\gamma} U_{\gamma\delta} = \mu_{\alpha} \delta_{\alpha\delta}$$

and defining the orthonormal Liouville space vectors

$$|c_{\alpha}\rangle = \sum_{\beta} |A_{\beta}\rangle U_{\beta\alpha}$$

and

$$|I_{\alpha}\rangle = \frac{1}{\sqrt{\mu_{\alpha}}} \sum_{\beta\gamma} U_{\alpha\beta}^+ f_{\beta\gamma} |B_{\gamma}\rangle$$

then the expansion of F becomes

$$F = \sum_{\alpha} \sqrt{\mu_{\alpha}} |c_{\alpha}\rangle \otimes |I_{\alpha}\rangle \quad (\text{A-1})$$

It can be immediately verified that, whenever F is idempotent as an operator in state-vector space (i.e., associated to a pure state), one has (cf. eq. (I-1))

$$\sqrt{\mu_{\alpha}} = \alpha_i \alpha_j \quad (\text{for } \alpha \equiv i, j)$$

this implies a complete equivalence of the Liouville space and the state-vector space Schrödinger decompositions in this case. Eq. (A-1) is however more general, as it applies to situations in which

F describes a mixture. In particular, whenever $F' = 0$ in the decomposition utilized in section II

$$F = R\rho + F'$$

we see that F is already in form (A-1) with a single nonvanishing coefficient μ_{α} . Note that either or both R and ρ can be von Neuman mixtures.

A decomposition of the Liouvillian dynamics given by

$$i\dot{F} = [H, F] \equiv LF$$

can be obtained, using eq. (A-1), in a way which is entirely parallel to the corresponding procedure in state vector space. Defining subsystem Liouvillian generators as

$$i\dot{|c_{\alpha}\rangle} = \ell_{\alpha} |c_{\alpha}\rangle \quad \text{and} \quad i\dot{|I_{\alpha}\rangle} = \ell_I |I_{\alpha}\rangle$$

we are led to (cf. eqs. (I-8) to (I-10))

$$\mu_{\beta}^{1/2} [(c_{\beta} | \ell_c | c_{\beta}) + (I_{\beta} | \ell_I | I_{\beta})] = \text{Re} (c_{\beta} I_{\beta} | L | F) \quad (\text{A-2})$$

$$\frac{d}{dt} \mu_{\beta}^{1/2} = \text{Im} (c_{\beta} I_{\beta} | L | F) \quad (\text{A-3})$$

$$\begin{aligned} (\mu_{\alpha}^{1/2} \pm \mu_{\beta}^{1/2}) [(I_{\beta} | \ell_I | I_{\alpha}) \pm (c_{\alpha} | \ell_c | c_{\beta})] = \\ = (I_{\beta} c_{\alpha} | L | F) \pm (F | L | I_{\alpha} c_{\beta}) \end{aligned} \quad (\text{A-4})$$

Note that eqs. (A-4) hold for $\alpha \neq \beta$.

APPENDIX B

DEGENERATE OCCUPATION PROBABILITIES AND THE SCHRÖDINGER DECOMPOSITION

When a number of coefficients in eq. (I-1) are equal, say, $\alpha_1 = \alpha_2 = \dots = \alpha_M = \bar{\alpha}$ it follows at once that the form of that decomposition is preserved if the associated natural states $|c_i\rangle$ and $|I_i\rangle$ ($i=1, \dots, N$) are transformed according to

$$|\tilde{c}_i\rangle = \sum_j u_{ij} |c_j\rangle \quad ; \quad |\tilde{I}_i\rangle = \sum_j u_{ij}^* |I_j\rangle$$

$\{u_{ij}\}$ being a $N \times N$ unitary matrix. Indeed, unitarity of u suffices to show that

$$\sum_{i=1}^N \alpha_i |c_i I_i\rangle = \bar{\alpha} \sum_{i=1}^N |c_i I_i\rangle = \bar{\alpha} \sum_{i=1}^N |\tilde{c}_i \tilde{I}_i\rangle$$

This freedom in the choice of natural states with degenerate occupation probabilities can be used to fulfill the conditions

$$\langle \tilde{c}_i \tilde{I}_j | H | \psi \rangle - \langle \psi | H | \tilde{c}_j \tilde{I}_i \rangle = 0 \quad ; \quad i, j = 1, \dots, N \quad (B-1)$$

so that the right hand side (with the lower sign) of eq. (I-8) is made to vanish. This avoids singular behavior of the corresponding matrix elements of the hermitean generators h_c and h_I in a way akin to the handling of vanishing energy denominators in standard, low order perturbation theory.

In order to further determine the matrix elements of h_c and h_I within the degenerate subspace one may perturb equal occupation amplitudes α_i and α_j to obtain, in terms of the states $|\tilde{c}_i\rangle$ and $|\tilde{I}_i\rangle$ satisfying eq. (B-1),

$$\begin{aligned} 2 \left[\langle \tilde{I}_j | h_I | \tilde{I}_i \rangle - \langle \tilde{c}_i | h_c | \tilde{c}_j \rangle \right] &= \\ &= \langle \tilde{c}_i \tilde{I}_j | H | \tilde{c}_i \tilde{I}_i - \tilde{c}_j \tilde{I}_j \rangle - \langle \tilde{c}_i \tilde{I}_i - \tilde{c}_j \tilde{I}_j | H | \tilde{c}_j \tilde{I}_i \rangle \end{aligned} \quad (B-2)$$

which, together with the expression for the sum of the same two matrix elements, on the left-hand side can be solved for each one of them. Note that these relations explicitly guarantee the hermitean character of h_c and h_I .

The degeneracy of all states in the null spaces of the reduced densities R and ρ (i.e., states with vanishing occupation) also deserves some comments. Since for these states both signs in eq. (I-8) give a vanishing left-hand side, it follows that, for $i \neq j$ (and $\alpha_i = \alpha_j = 0$) one must have

$$\langle c_i I_j | H | \psi \rangle = 0 \quad (B-3)$$

This can be used to determine the appropriate representation for the null space (or for the relevant subspace of it, at least) as follows. First construct the doorway

$$N P_0 H | \psi \rangle = | D_0 \rangle$$

where N is a normalization factor, and P_0 projects onto the product of the null subspaces of R and ρ . Then consider the Schrödinger decomposition of $| D_0 \rangle$.

$$| D_0 \rangle = \sum_i d_i | c_i I_i \rangle$$

where now $|c_i\rangle$ and $|I_i\rangle$ lie in the null spaces of the respective densities. These states will then naturally and sufficiently extend the set of natural states associated with nonvanishing

occupations in the sense that they automatically fulfill eq. (B-3) and span the full subspace that can be reached by letting H act on $|\psi\rangle$.

REFERENCES

- (1) C.Y. Wong and H.H.K. Tang, Phys. Rev. Lett. 40, 1070 (1978).
- (2) H. Orland and R. Schaeffer, Nucl. Phys. A,
- (3) S. Ayik, Zeit. für Phys. 298, 83 (1980).
- (4) P. Grangé, H.A. Weidenmüller, G. Wolschin, preprint MPI H-1981-V8.
- (5) R. Balian, M. Veneroni, Saclay preprint, DPH-T-81-017.
- (6) A.F.R. de Toledo Piza, preprint IFUSP/P-275 (1981).
- (7) D. Agassi, C.M. Ko, H.A. Weidenmüller, Ann. Phys. (N.Y.), 107, 140 (1977).
- (8) R.A. Broglia, C.H. Dasso, A. Winther, Nordita preprint 80/16.
- (9) E. Schrödinger, Proc. Camb. Phil. Soc. 31, 555 (1935).
ibid. 32, 446 (1936).
- (10) E. Schmidt, Math. Annalen 63, 433 (1907).
- (11) M. Reed and B. Simon, Methods of Modern Mathematical Physics, vol. I, Academic Press, N.Y. (1972), pg. 203.
- (12) O. Kübler, H.D. Zeh, Ann. Phys. (N.Y.) 76, 405 (1973).
- (13) M.C. Nemes, preprint MPI-H (1981) V-11 - to be published in Nucl. Phys. A.
- (14) P.C. Lichtner, J.J. Griffin, Phys. Rev. Lett. 37, 1521 (1976).
- (15) C.R. Willis, R.H. Picard, Phys. Rev. A9, 1343 (1974).
- (16) H. Esbensen, A. Winther, R.A. Broglia, C.H. Dasso, Phys. Rev. Lett. 41, 296 (1978).
- (17) H. Esbensen, Nordita preprint 79/45.
- (18) S.R. de Groot and L.G. Suttrop, Foundation of Electrodynamics, North-Holland Publ. Co., Amsterdam, 1972, p. 341.
- (19) F. John, Partial Differential Equations, Springer-Verlag (1975).