BEYOND THE TIME-DEPENDENT HARTREE-FOCK:

The collision terms in a mean-field theory.

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Abstract: (1) A many-body Hamiltonian is proposed, for which TDHF constitutes a rigorous solution. This allows to define a residual interaction appropriate for TDHF. (2) The impact of the residual interaction is studied in a non-perturbative approximation and without ensemble averages. (3) The further reduction to the one-body level is possible without ad hoc assumptions, and produces a closed equation of motion for the one-body density. (4) The residual interaction causes a collision term which acts simultaneously on intrinsic and on collective motion.

At this conference, we have heard on the many facets of the time-dependent Hartree-Fock equations, on their beauty of producing almost parameter-free results, and on their success in comparison with the experimental data. But even more than forty years after their first formulation by Dirac |1|, it is not perfectly clear - at least not to me - what type of approximation they stand for vis à vis the full quantum-mechanical many-body problem, and because of this, it is unclear, how and in which sense one could go "beyond" this formalism.

In this short lecture I cannot give a review or even comment on the numerous attempts of this kind |2 - 14|, rather shall I concentrate on some aspects of the problem, as they were published by Mantzouranis and myself |11| or were laid down in a recent series of preprints |12 - 14|.

In presenting my arguments I shall put weight on the following four questions. 1. Does a physical problem, does a Hamiltonian exist, to which TDHF is a rigorous solution ? 2. Can one treat a suitably defined residual interaction <u>without</u> perturbation theory of finite order or <u>without</u> using the method of ensemble averages ? 3. Can one reduce the equations of motion for the A-body density to those for the one-body density without using the idempotency condition at any stage? and 4. Are the modifications of the TDHF-equations - the terms beyond

TDHF - are they relevant in any physical context ?

For to be specific, I discuss a closed system of A fermions which move subject to their pairwise interaction $\tilde{V}$. This system is defined by the Hamiltonian $\tilde{H}$

$$\tilde{H} = \sum_{m_1,m_2} \langle m_1|K|m_2\rangle a^+_{m_1} a_{m_2} + \frac{1}{4}\sum_{m_1,m_2..m_4} \langle m_1,m_2|\tilde{V}|m_3,m_4\rangle a^+_{m_2} a^+_{m_1} a_{m_3} a_{m_4} . \quad (1)$$

I aim at the solution of the time-dependent state $|t\rangle$, i.e. $(\tilde{H} - i\hbar \frac{d}{dt})|t\rangle = 0$, or more specifically at an appropriate solution of the A-body density operator $\tilde{M}(t) = |t\rangle\langle t|$ by means of

$$i\hbar\, d/dt\, \tilde{M}(t) = [\tilde{H}, \tilde{M}(t)] . \quad (2)$$

In the lack of a rigorous solution, one must approach this problem by a kind of perturbative approach. One defines a soluble Hamiltonian H , whose time-dependent amplitudes $|\mu(t)\rangle$,

$$(H - i\hbar\, d/dt)|\mu(t)\rangle = 0 \quad (3)$$

provide us with a complete set of states (the Hilbert space) for a systematic discussion of the "residual interaction V_S" which is defined by

$$\tilde{H} = H + V_S \quad (4)$$

One is tempted to identify the unperturbed states $|\mu(t)\rangle$ with the TDHF solutions. This, at least, would be intuitively appealing. However, one realises immediately that TDHF is defined by a one-body operator $h_{HF}(t)$; the Hamiltonian on the A-body level is largely unknown. The most straightforward identification, $H_w = \sum_i h_{HF}(i)$ cannot be correct by two reasons: 1) H_w and H do not have the same energy, they differ by half the interaction energy; 2) The so defined H_w has only one many-body state as a rigorous solution $(H_w - i\hbar\, d/dt)\ |\mu_o(t)\rangle = 0$, and not a complete set.

Some time ago, Mantzouranis and myself |10| have proposed another unperturbed Hamiltonian H

$$H = \sum_{m_1,m_2} \langle m_1(t)|K|m_2(t)\rangle a^+_{m_1} a_{m_2} - \frac{1}{2}\sum_{m_1,m_2} \langle m_1(t),m_2(t)|\tilde{V}|m_1(t),m_2(t)\rangle a^+_{m_1} a_{m_1} a^+_{m_2} a_{m_2} + \sum_{m_1,m_2,m} \langle m_1(t), m(t)|\tilde{V}|m_2(t),m(t)\rangle a^+_{m_1} a_{m_2} a^+_{m} a_{m} . \quad (5)$$

By definition, this genuine two-body operator cannot cause more than zero or one-particle-one-hole excitations, when acting on an arbitrary state $|\mu(t)>$. The one-body amplitudes can be set zero by properly choosing the time-derivative of single-particle states $|m(t)>$. This condition leads straightforward to

$$i\hbar\, d/dt\ |m(t)> = h^{(\mu)}(t)\,|m(t)>. \tag{6}$$

The time-dependent one-body operator $h^{(\mu)}(t)$,

$$<m_i|h^{(\mu)}|m_j>=<m_i(t)|K|m_j(t)> + \sum_m p_m(t)<m_i(t),m(t)|V|m_j(t),m(t)> \tag{7}$$

looks formally like the TDHF Hamiltonian, but the state-dependent occupation numbers

$$p_m^{(\mu)}(t) = <\mu(t)|a_m^+(t)\ a_m(t)|\mu(t)> \tag{8}$$

defined as the probability to find state $|m(t)>$ occupied in the many-body state $|\mu(t)>$ need not be zero or one by necessity, as in the familiar theories.

Thus, one has found an answer to the first question: The TDHF equations are a rigorous solution to the Hamiltonian H as given by Eq. (5).- Simultaneously one has found that part of the full Hamiltonian H which by definition cannot be included in TDHF, the residual interaction V_S. It is defined rigorously by $V_S = \tilde{H} - H$, and thus by

$$\begin{aligned} V_S = \frac{1}{4} \sum_{m_1,m_2,m_3,m_4} & <m_1,m_2|\tilde{V}|m_3,m_4>a_{m_2}^+ a_{m_1}^+ a_{m_3} a_{m_4} \\ - \sum_{m_1,m_2,m_3} & <m_1,m_2|\tilde{V}|m_3,m_2>a_{m_2}^+ a_{m_1}^+ a_{m_3} a_{m_2} \\ + \frac{1}{2} \sum_{m_1,m_2} & <m_1,m_2|\tilde{V}|m_1,m_2>a_{m_2}^+ a_{m_1}^+ a_{m_1} a_{m_2} \end{aligned} \tag{9}$$

The operator V_S has no diagonal elements in between the Hartree-Fock states, i.e. $<\mu(t)|V_S|\mu(t)> = 0$, and can generate only two-particle-two-hole amplitudes when applied to any $|\mu(t)>$.

We proceed now to the second question: How can we incorporate the residual interaction - i.e. those terms beyond TDHF - at least approximately ? - As usually, the problem can be treated further in interaction representation. The solutions to the unperturbed problem Eq. (3), defines a set of complete states $|\mu(t)\rangle$, which can be understood as a unitary transformation of the initial states $|\mu(0)>$, i.e. $|\mu(t)> = U(t)|\mu(0)>$. The unitary operators can be used to define $V(t) = U^+(t)\ V_S(t)\ U(t)$ and $N(t) = U^+(t)M(t)U(t)$.

Then, Eq. (2) is replaced quite straightforwardly by

$$i\hbar\, d/dt\, N(t) = [V(t), N(t)] \quad . \tag{10}$$

Its formal solution

$$N(t) = N(0) + \frac{1}{i\hbar}\int_0^t ds\,[V(s), N(s)] \tag{11}$$

is treated in a somewhat unconventional way. The Hilbert space is defined by the unperturbed problem, and therefore it makes sense to divide $N(t)$ into its diagonal part $N_D(t)$ and its off-diagonal parts $N_S(t)$, which obey a set of coupled equations

$$N_D(t) = N_D(0) + \frac{1}{i\hbar}\int_0^t ds\,[V(s), N_S(s)] \quad , \text{ and}$$

$$N_S(t) = N_S(0) + \frac{1}{i\hbar}\int_0^t ds\,[V(s), N_D(s)] + \frac{1}{i\hbar}\int_0^t ds\,[V(s), N_S(s)]. \tag{12}$$

This couple of equations can be analysed in the following way. For a given operator function $N_S(t)$, the diagonal elements are determined as a simple quadrature and this way are fixed. Opposed to this, for a given $N_D(t)$, the second equations remains an integral equation for $N_S(t)$ and can be formally solved by an infinite series. Retaining the lowest non-trivial terms (we call it the approximation of rank zero) one has for a diagonal initial state $N(t_o) = N_D(t_o)$

$$d/dt\, N_S(t) = \frac{1}{i\hbar}[V(t), N_D(t)] \tag{13}$$

$$d/dt\, N_D(t) = -\frac{1}{\hbar^2}\int_0^t ds\,[V(t),[V(s), N_D(s)]]. \tag{14}$$

In other words, the diagonal elements are determined from a closed (integral) equation; once $N_D(t)$ is known, one can determine the off-diagonal $N_S(t)$. - In a series of preprints |12-14| , I have carefully investigated whether the restriction to rank zero can do any harm ot introduce inconsistencies; it does not. Needless to say, that particle number and energy are conserved.

The procedure indicated above corresponds to an infinite series in conventional perturbation theory. Rewriting equation as an integral equation, one has for example

$$N_D(t) = N_D(t_o) + \left(\frac{1}{i\hbar}\right)^2 \int_0^t ds_1 \int_0^{s_1} ds_2\, [\overbrace{V(s_1),[V(s_2),N_D(t_o)]}]$$

$$+ \left(\frac{1}{i\hbar}\right)^4 \int_0^t ds_1 \int_0^{} ds_2 \int_0^{} ds_3 \int_0^{s_3} ds_4\, [\overbrace{V(s_1),[V(s_2),[\overbrace{V_S(s_3),[V(s_4)N(t_o)]}]]}]$$

$$+ \ldots \tag{15}$$

for the diagonal elements, and a similar equation for the off-diagonal

elements. In other words: Out of the infinite series of conventional perturbation theory, the above procedure picks out those graphs which contain an even power of interactions $V(t)$, and among them only those which are contracted pairwise and sequentially in time. This is the same series as one would have obtained with a suitably defined ensemble average over a Gaussian distribution of matrix elements.

I should conclude this section with the remark that I consider Eq.(14) as an approximation to the exact equation for the actual system of particles rather than an exact solution for an ensemble of systems. Conceptually, both concepts are very different from each other, but I do not intend to deepen this point in the present context.

Last but not least, we can assume that the diagonal elements $P_\mu(t) = \langle\mu|N_D(t)|\mu\rangle$ change with time slower than the rapidly oscillating functions $\langle\mu|V(t)|\mu'\rangle$. The argument of N_D in Eq. (14) under the integral can thus be replaced by its value at the upper integration limit, i.e.

$$N_D(t) = -\frac{1}{\hbar^2}\int_0^t ds\,[V(t),[V(s),N_D(t)]] \quad . \tag{16}$$

I have verified elsewhere |12| that this substitution is consistent within the lowest rank of approximation. - We have thus found an answer to question number 2 and can proceed with the reduction to the one-body problem.

The reduction to the one-body level is more or less straightforward and yields in normal representation

$$d/dt\ p_{m_1} = -\sum_{m_2,m_3,m_4} w(m_1,m_2,m_3,m_4;t)\{p_{m_1}p_{m_2}(1-p_{m_3})(1-p_{m_4}) - (1-p_{m_1})(1-p_{m_2})\,p_{m_3}\,p_{m_4}\} \tag{17}$$

This equation associates the change per unit time of the one-body occupation numbers, as defined by Eq. (8), with their value at the actual time t in terms of the matrix elements of the residual interaction, which are condensed into the time-dependent transition rates w, i.e.

$$w(m_1,m_2,m_3,m_4;t) = \frac{1}{\hbar^2}\int_0^t ds\ \langle m_1(t), m_2(t)|V|\ m_3(t)m_4(t)\rangle \cdot \cdot \langle m_3(s),m_4(s)|V|m_1(s)m_2(s)\rangle \quad + \text{c.c.} \tag{18}$$

Together with the generalised TDHF-equations Eq. (6) and (7), the

latter represent a set of coupled integro-differential equations for the self-consistent determination of the amplitudes $|m(t)>$ and their occupation $p_m(t)$. All these equations, Eqs. (6-8) and (17-18), can be cast into the compact form

$$\dot{\rho} = \frac{1}{i\hbar}[h_{HF}(t), \rho(t)] + C[\rho] \tag{19}$$

which related the change per unit time of the one-body density operator $\rho(t)$ to the density at the actual time. The first of the two terms on the r.h.s. represents the usual TDHF commutator, the second term $C[\rho]$,

$$C[\rho] = \sum_m |m(t)> \dot{p}_m(t) <m(t)| \tag{20}$$

represents all what is"beyond TDHF".In the present approximation, the operator C has a structure like the "collisions terms in the Boltzmann equation".

The reduction to the one-body level involves one type of approximation which should be outlined in short. Primarily, in the reduction, $\dot{p}_m(t)$ is a functional of the diagonal elements of the two- and of the three-body density, $p_{m_1,m_2}(t)$ and $p_{m_1,m_2,m_3}(t)$, respectively. They appear in characteristic combinations with the transition rates $w(m_1m_2m_3m_4,t)$. These transition rates are kind of absolute squares with respect to the quantum numbers m_i, and therefore vary smoothly with any of the four, the other three being fixed. One is thus entitled to the following type of substitution

$$\sum_{m_3} w(m_1,m_2,m_3,m_4;t)\ p_{m_1m_2m_3}(t)$$
$$\sim \frac{1}{6}\ p_{m_1m_2}(t) \sum_{m_3} w(m_1,m_2,m_3,m_4;t)\ \ p_{m_3}(t) \tag{21}$$

and this gives directly Eq. (17). The structure of Eq. (17) is caused by the nature of the residual interaction and the way they enter into the formalism. It is not a property of the density matrices. In fact, a factorisation of the three-body density into a product of one-body matrices would be inconsistent within the formalism.

So far we have concentrated on the formal aspects of the problem. In view of the rather weak assumptions made - restriction to the lowest rank (I) and smoothness of transition rates (II) - we must conclude that terms beyond TDHF are doubtlessly present and in their crudest approximation can be formulated by collision terms in a self-consistent fashion.

We arrive thus at our fourth and last question: "Collision terms are present, but are they relevant in any physical context?" - The answer to this question cannot be given in generality, because the unperturbed TDHF states depend drastically on the initial condition. However we can discuss two particular, realistic cases.

(1) The quasistationary case: Suppose, the initial configuration corresponds to a stationary Hartree-Fock solution with eigenstates $|m\rangle$ and single-particle states ε_m. The time-dependent amplitudes are then given by $|m(t)\rangle = |m\rangle \exp(-i\varepsilon_m t/\hbar)$. In this case the time-dependent transition rates can be easily evaluated and yield

$$w(m_1,m_2,m_3,m_4;t) = \frac{1}{\hbar}\delta(\varepsilon_{m_1} + \varepsilon_{m_2} - (\varepsilon_{m_3} + \varepsilon_{m_4}))\,|\langle m_1,m_2|V_S|m_3,m_4\rangle|^2$$

After some 10^{-24} seconds the time-dependent phases settle into a constant, producing essentially the energy conserving δ-function. Thus, by virtue of the residual interaction, transitions between any pair of single-particle states are possible only if the single-particle energies match: $\varepsilon_{m_1} + \varepsilon_{m_2} = \varepsilon_{m_3} + \varepsilon_{m_4}$. If the initial occupation has been chosen such that all energy levels up to a certain energy, (the Fermi energy ε_F), are occupied and all others are empty ($p_m = 0$), the residual interaction cannot cause transitions by lack of phase space. In other words: The non-degenerate Hartree-Fock ground state is stationary and not affected by the residual interaction. If, however, the initial occupation allows for transition at the same energy, the system will equilibrate to an equilibrium occupation

$$p_m = e^{-(\varepsilon_m - \varepsilon_F)/kT}$$

within the equilibration time. Both, very rough estimates as well as the more detailed calculation of Wolschin |8| produce equilibration times of a few times 10^{-23} seconds for realistic cases. -

(2) The heavy-ion collision or coherent motion:
The above considerations disregard like most of the actual calculations |2-11| the impact of collective motion. The latter is of particular importance in a heavy-ion collision, which shall be sketched in short. Prior to the collision, the TDHF solutions for a time-dependent single-particle state $|m(t)\rangle$ have the structure

$$\langle x|\ m(t)\rangle = \langle x - \xi(t)|m\rangle\ e^{i(k\cdot x - \omega_m t)}$$

in configuration space with

$$\hbar\omega_m = \varepsilon_m - (\hbar k)^2/2m$$

These wave functions reflect the fact that the TDHF-nucleus travels through space on the collective trajectory $\xi(t) = \hbar kt/m + \xi(0)$ with the collective momentum $\hbar k$. Assuming for the moment a straightline trajectory for all times, the time-dependent transition rate w can be evaluated, with the result

$$w(m_1,m_2,m_3,m_4;t) = \delta(\varepsilon) \cdot F(t) \ .$$

The function $F(t)$ is given elsewhere in detail |13| and changes slowly in time; it differs from zero essentially only when the ions are in contact. More important is the δ-function in front of F. Its argument has the structure

$$\varepsilon = (\varepsilon_{m_1} + \varepsilon_{m_2} - \varepsilon_{m_3} - \varepsilon_{m_4}) + \frac{\hbar^2}{4m}(k_1-k_2)^2 - \frac{\hbar^2}{4m}(k_3-k_4)^2$$

This displays visibly the important and novel property of the present rather rigorous approach. Transitions are possible not only between different intrinsic states $|m\rangle$ with the same collective momentum, but also between states of different collective momentum. With other words: The residual interaction can cause intrinsic excitation with its characteristic spread over many single-particle states, but simultaneously it causes collective excitations with a characteristic spread over many trajectories. The initial, sharp TDHF trajectory gets transformed during the time of contact into a bundle of TDHF trajectories. A formalism "Beyond TDHF" can thus eventually account for the large variances of collective variables like c.m. position, angle or mass, which seem to appear in the experimental cross section and which so far were impossible to obtain in TDHF calculations without "collision terms".

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