Mean Field Methods for Atomic and Nuclear Reactions: The Link between Time–Dependent and Time–Independent Approaches

J. Uhlig, J. C. Lemm and A. Weiguny
Institut für Theoretische Physik I
Universität Münster
D–48149 Münster, Germany

PACS: 03.65.Nk; 24.10.-i; 34.10.+x

Abstract

Three variants of mean field methods for atomic and nuclear reactions are compared with respect to both conception and applicability: The time–dependent Hartree–Fock method solves the equation of motion for a Hermitian density operator as initial value problem, with the colliding fragments in a continuum state of relative motion. With no specification of the final state, the method is restricted to inclusive reactions. The time–dependent mean field method, as developed by Kerman, Levit and Negele as well as by Reinhardt, calculates the density for specific transitions and thus applies to exclusive reactions. It uses the Hubbard–Stratonovich transformation to express the full time–development operator with two–body interactions as functional integral over one–body densities. In stationary phase approximation and with Slater determinants as initial and final states, it defines non–Hermitian, time–dependent mean field equations to be solved self–consistently as boundary value problem in time. The time–independent mean field method of Giraud and Nagarajan is based on a Schwinger–type variational principle for the resolvent. It leads to a set of inhomogeneous, non–Hermitian equations of Hartree–Fock type to be solved for given total energy. All information about initial and final channels is contained in the inhomogeneities, hence the method is designed for exclusive reactions. A direct link is established between the time–dependent and time–independent versions. Their relation is non–trivial due to the non–linear nature of mean field methods.

1 Similarities and Differences

After the success which mean field methods have had for bound state problems in various fields of physics, it was only natural to try the mean field concept for scattering states as well. The original attempt in this direction is the time–dependent Hartree–Fock method (TDHF) developed about 20 years ago [1]. In this method one solves the equation of motion for the one–body density operator $\rho = \rho(t)$,

$$i\hbar \frac{\partial}{\partial t} \rho = [h, \rho] \; , \tag{1.1}$$

with an <u>initial</u> condition for ρ,

$$\rho(t_i) = \rho_i \; , \tag{1.2}$$

describing an unbound state of relative motion of the colliding fragments. The density operator ρ can be represented in just <u>one</u> basis of single–particle states $\psi_m(t)$,

$$\rho = \sum_{m=1}^{N} \mid \psi_m(t) >< \psi_m(t) \mid \tag{1.3}$$

for N particles and with $\psi_m(t)$ orthonormalized. The single–particle Hamiltonian h is Hermitian and has standard Hartree–Fock structure, $h = t + u$ with mean field potential

$$u = \sum_{m=1}^{N} < \cdot\, \psi_m(t) \,|\, v \,|\, \cdot\, \psi_m(t) > \; , \tag{1.4}$$

where the dots represent wave functions of some arbitrary single–particle basis. The single–particle states $\psi_m(t)$ are determined from the time–dependent Hartree–Fock equations

$$i\hbar \frac{\partial}{\partial t} \,|\, \psi_m(t) > = h \,|\, \psi_m(t) > \tag{1.5}$$

with initial conditions

$$\psi_m(t_i) = \chi_m \qquad \text{for } m = 1, 2, \ldots N \; . \tag{1.6}$$

Standard manipulation of eq. (1.5) and its Hermitian adjoint leads to eq. (1.1), with initial condition (1.2) corresponding to (1.6). In practice, the non–linear equations (1.1) and (1.5), respectively, are solved by iteration: A set of N occupied orbitals is used to compute the potential u. With the corresponding solutions of (1.1) or (1.5) one recalculates u till self–consistency is reached. As each iteration step requires as input only the set of N functions ψ_m at fixed time t, the TDHF method as initial value problem is "local" in time.

From the densities $\rho_b(\vec{r}, t)$ according to (1.1) and (1.2), taken at various classical impact parameters b, one may calculate a classical cross section. Although it can generate nice snapshots of the density distribution during the scattering process, the method has two problems: First, as initial value problem it can at best handle inclusive reactions, since no specification of a final channel enters the formalism. The second, more serious problem concerns "spurious cross channel correlations": Starting from the determinant $\Psi(t_i)$ corresponding to ρ_i the method generates a single determinant $\Psi(t)$. Due to the non–linear nature of the TDHF equations, this determinant $\Psi(t)$ continues to vary as time goes to infinity. Hence, if this wave function is expanded in an orthogonal set of channel wave functions, the expansion coefficients will not be constant asymptotically. Thus an S–matrix, constructed by projecting the TDHF wave functions onto channel wave functions, would not be constant in time [2].

The time–dependent mean field method (TDMF) [3, 4] also uses an equation of motion like (1.1),

$$i\hbar \frac{\partial}{\partial t} \rho \;=\; [h, \rho] \;, \tag{1.7}$$

however, there are two important differences:
1. The density operator ρ of (1.7) is expanded in <u>two</u> sets of mutually biorthogonal single–particle functions,

$$\rho \;=\; \sum_{m=1}^{N} \frac{|\,\psi_m(t)\;><\;\tilde{\psi}_m(t)\,|}{<\;\tilde{\psi}_m(t)\,|\,\psi_m(t)\;>} \;, \tag{1.8}$$

and the Hamiltonian $h \;=\; t \;+\; u$ with mean field potential

$$u \;=\; \sum_{m=1}^{N} \frac{<\cdot\,\tilde{\psi}_m(t)\,|\,v\,|\;\cdot\;\psi_m(t)\;>}{<\;\tilde{\psi}_m\,|\,\psi_m\;>} \tag{1.9}$$

is <u>non</u>–Hermitian in general.
2. Eq.(1.7) has to be solved self–consistently as <u>boundary</u> problem in time t, fixing

$$\rho(t_i) \;=\; \rho_i \quad \text{and} \quad \rho(t_f) \;=\; \rho_f \;. \tag{1.10}$$

The single–particle functions $\psi_m(t)$ are obtained from

$$i\hbar \frac{\partial}{\partial t} |\,\psi_m(t)\;> \;=\; h\,|\,\psi_m(t)\;> \tag{1.11}$$

by forward propagation of initial wave functions

$$\psi_m(t_i) \;=\; \chi_m \qquad \text{for} \;\; m \;=\; 1,\, 2,\, \ldots N \;. \tag{1.12}$$

Analogously $\tilde{\psi}_m(t)$ results from

$$-\,i\hbar \frac{\partial}{\partial t} \;<\;\tilde{\psi}_m(t)\,|\; =<\;\tilde{\psi}_m(t)\,|\,h \tag{1.11'}$$

by backward propagation of

$$\tilde{\psi}_m(t_f) \;=\; \chi_m^{'} \qquad \text{for} \;\; m \;=\; 1,\, 2,\, \ldots N \;. \tag{1.12'}$$

Combining (1.11) and (1.11') in the usual way, one obtains (1.7) with conditions (1.10) from (1.12), (1.12'). One also proves easily that

$$\frac{\partial}{\partial t} \;<\;\tilde{\psi}_m|\,\psi_n\;> \;=\; 0 \;, \tag{1.13}$$

hence if $\tilde{\psi}_m$, ψ_n are chosen biorthogonal at $t = t_i$, they will remain so at any time. In general, $\tilde{\psi}_m$ and ψ_m will be not complex–conjugate to each other, and ρ will be non–Hermitian. Only when $\chi_m^{'}$ is generated from χ_m by the mean field time development operator $U_h\,(t_f - t_i)$, we have $\tilde{\psi}_m\,(t) = \psi_m^*\,(t)$ in which case TDMF reduces to TDHF with just one set of single–particle functions. Equations (1.7), (1.10) as well as the coupled equations (1.11), (1.11') together with (1.12), (1.12') constitute a boundary condition problem in which the time plays a role similar to that of the spatial coordinates [5].

In practice, one may try to solve this problem self–consistently in analogy to the static Hartree–Fock problem by iteration [5] which involves an initial guess of the single–particle functions $\tilde{\psi}_m\,(t)$, $\psi_m\,(t)$ for <u>all</u> times t between t_i and t_f. In this sense, the TDMF boundary condition problem is highly "non–local" in the variable t. Since initial <u>and</u> final states are taken care of, the method is able to describe also exclusive reactions: Each quantum process, leading from given initial state χ to some final state $\chi^{'}$, has its own time–dependent mean field assigned. It has been proven [2] that, within the framework of TDMF, an S–matrix can be defined which becomes asymptotically constant. The problem with the TDMF approach lies in the above non–locality in time, for which there seems to exist no practicable algorithm for actual numerical calculations of (3 + 1)–dimensional systems.

Some comments on the lack of Hermiticity of ρ and of $h\,(\rho)$ are in order. This non–Hermitian structure is of a special type which preserves the usual properties of a single–particle density matrix connected to a Slater determinant. From the explicit expression (1.8) we have immediately

$$\mathrm{Tr}\,\rho = N \qquad \text{and} \qquad \rho^2 = \rho\;, \tag{1.14}$$

hence particle number is fixed and ρ is a projector on the space of occupied orbitals. Moreover, $|\,\psi_m >$ and $< \tilde{\psi}_m|$ are right and left eigenstates of ρ,

$$\rho\,|\,\psi_m\,(t) > = N_m\,|\,\psi_m\,(t) >\;;\; < \tilde{\psi}_m\,(t)\,|\,\rho = < \tilde{\psi}_m\,(t)\,|\,N_m \tag{1.15}$$

with eigenvalues

$$N_m = \begin{cases} 1 & \text{for } m \text{ occupied} \\ 0 & \text{otherwise} \end{cases} \;. \tag{1.16}$$

The eigenvalues of $h\,(\rho)$ will be complex in general, hence ψ_m and $\tilde{\psi}_m$ correspond to quasi–particles of finite lifetime. They represent intermediate states which the system passes during the reaction process. The S–matrix of the mean field approach will always violate unitarity, irrespective of the fact whether $h\,(\rho)$ is Hermitian or not: The $\mathcal{S}$–operator depends on ρ which in turn depends on the initial and final states of a specific reaction as mentioned above. Each quantum process $\chi \rightarrow \chi^{'}$ has its own mean field, calculated without reference to any other possible process.

An alternative to TDMF is the time–independent mean field method (TIMF) based on a Schwinger–type variational principle [6, 7] as described below in section 2. Like TDMF it uses <u>two</u> sets of variational functions and leads to a set of inhomogeneous equations for the single–particle functions $\varphi_i^{'}$, φ_i which may be chosen biorthogonal. The corresponding density operator

$$\rho \, = \, \sum_{i=1}^{N} \frac{| \, \varphi_i > < \varphi_i^{'} \, |}{< \varphi_i^{'} \, | \, \varphi_i >} \tag{1.17}$$

obeys an inhomogeneous equation,

$$[h, \rho] \, = \, \overline{\eta} \, (\rho_{\chi'} \, - \, \rho_{\chi}) \quad ; \quad \overline{\eta} \, = \, E \, - \, \frac{< \phi' \, | \, H \, | \, \phi >}{< \phi' \, | \, \phi >} \, , \tag{1.18}$$

where E is the total energy of the system, ϕ, $\phi^{'}$ are Slater determinants built from the single–particle functions φ_i, $\varphi_i^{'}$ and $\rho_{\chi'}$, ρ_{χ} are "mixed" densities containing all information about initial and final states χ, $\chi^{'}$. Hence the method can describe exclusive reactions. As in TDMF h is <u>non</u>–Hermitian,

$$h \, = \, \sum_{i=1}^{N} \frac{< \cdot \, \varphi_i^{'} \, | \, v \, | \, \cdot \, \varphi_i >}{< \varphi_i^{'} \, | \, \varphi_i >} \, , \tag{1.19}$$

but now of course time–independent as are the single–particle functions φ_i, $\varphi_i^{'}$. Their self–energies η_i are complex in general due to the lack of Hermiticity of h. As regards its practical applicability [8], TIMF is much simpler than TDMF: One has to solve inhomogeneous, complex equations of Hartree–Fock type at some given energy E. In this respect TIMF is comparable to TDHF: While TDHF is "local" in time, TIMF is "local" in energy.

In view of the above similarities and differences of time–dependent and time–independent mean field methods (see table 1), it appears desirable to establish a direct link between TDMF and TIMF. Their relation is non–trivial due to the non–linear nature of mean field methods.

The paper is organized as follows: In section 2 we shall derive matrix elements of the resolvent operator as stationary values of a Schwinger–type functional in mean field approximation. Its stationarity conditions are given by the TIMF equations (1.17) and (1.18). To calculate matrix elements of the exact time–development operator we use a path integral representation based on the Hubbard–Stratonovich transformation (section 3). Ambiguities of the respective auxiliary fields σ are briefly discussed in section 4, following [9]. The mean field approximation of the time–development operator is then obtained by applying the stationary phase approximation to the path integrals over the auxiliary fields σ in section 5. The result is the boundary condition problem for ρ, eqs. (1.7) to (1.10), of the TDMF method. The link between the two methods is obtained in two steps: First, in static approximation of TDMF (section 6) we can introduce single–particle propagators $g_m \, = \, (w_m \, - \, h(\sigma))^{-1}$ by Fourier transformation of the corresponding time–development operator $\exp \{ - \, \frac{i}{\hbar} \, h(\sigma) \, T \}$. Second, the Fourier integrals over w_m are solved in stationary phase approximation on the same footing (section 7) as the path integrals over the static auxiliary fields σ. Thus the integrals over real variables w_m are replaced by the integrand at some complex values ω_m° which are identified in section 9 as the self–energies η_m of TIMF after the T–integration has been carried out (section 8). At the same time one reproduces the TIMF value of the resolvent. In conclusion (section 9): TIMF turns out to be a static approximation of TDMF in semi–classical approximation.

2 Resolvent operator in mean field approximation

The TIMF method solves the stationarity equations of a functional like [6, 7]

$$F(\Psi', \Psi) = <\chi'|\Psi> + <\Psi'|\chi> - <\Psi'|(E-H)|\Psi> \tag{2.1}$$

which read

$$(E-H)|\Psi>= |\chi> \; ; \; <\Psi'|(E-H) = <\chi'| \tag{2.2}$$

with χ, χ' as initial and final states. The resolvent matrix element between χ and χ' is then given by

$$<\chi'|(E-H)^{-1}|\chi> = <\chi'|\Psi> = <\Psi'|\chi> \quad . \tag{2.3}$$

In mean field approximation one takes χ, χ' as Slater determinants,

$$\chi = \mathcal{A} \prod_{i=1}^{N} \chi_i \; ; \; \chi' = \mathcal{A} \prod_{i=1}^{N} \chi_i' \, , \tag{2.4}$$

and the variational functions Ψ, Ψ' are correspondingly restricted to Slater determinants as well,

$$\phi = \mathcal{A} \prod_{i=1}^{N} \varphi_i \; ; \; \phi' = \mathcal{A} \prod_{i=1}^{N} \varphi_i' \, . \tag{2.5}$$

The antisymmetrizer $\mathcal{A}$ is defined as $\mathcal{A} = (N!)^{-\frac{1}{2}} \sum_P (-)^P P$. One then has to vary

$$F(\phi', \phi) = <\chi'|\phi> + <\phi'|\chi> - <\phi'|(E-H)|\phi> \quad . \tag{2.6}$$

To calculate $F(\phi', \phi)$ and its functional derivatives, one can use the invariance of the above four determinants under unitary transformation of their orbitals in order to diagonalize the four N–dimensional matrices $<\chi_i' \mid \varphi_j>$, $<\varphi_i' \mid \chi_j>$, $<\varphi_i' \mid \varphi_j>$ and $<\varphi_i' \mid h \mid \varphi_j>$. Here $h = t + u$ is the single–particle Hamiltonian with u the Hartree–Fock potential in the biorthogonal basis φ_i', φ_j. In this representation the stationarity equations of (2.6) read:

$$(\eta_i - h) \mid \varphi_i> = \lambda_i \mid \chi_i> \; ; \; <\varphi_i' \mid (\eta_i - h) = <\chi_i' \mid \lambda_i' \tag{2.7}$$

with complex self–energies

$$\eta_i = E - \frac{<\phi' \mid H \mid \phi>}{<\phi' \mid \phi>} + \frac{<\varphi_i' \mid h \mid \varphi_i>}{<\varphi_i' \mid \varphi_i>} \, . \tag{2.8}$$

The stationary value of $F(\phi', \phi)$ is then

$$F_{stat} = <\chi' \mid \phi> = <\phi' \mid \chi> = \prod_i \lambda_i <\chi_i' \mid g_i \mid \chi_i> = \prod_i \lambda_i' <\chi_i' \mid g_i \mid \chi_i> \tag{2.9}$$

with single–particle propagators

$$g_i = (\eta_i - h)^{-1} \, . \tag{2.10}$$

The explicit form of λ_i, $\lambda_i^{'}$ – which we shall need in the following – is

$$\lambda_i \;=\; \frac{<\phi^{'} \mid \chi>}{<\phi^{'} \mid \phi>} \cdot \frac{<\varphi_i^{'} \mid \varphi_i>}{<\varphi_i^{'} \mid \chi_i>} \;\;;\;\; \lambda_i^{'} \;=\; \frac{<\chi^{'} \mid \phi>}{<\phi^{'} \mid \phi>} \cdot \frac{<\varphi_i^{'} \mid \varphi_i>}{<\chi_i^{'} \mid \varphi_i>} \;. \tag{2.11}$$

They are related to each other and to $\overline{\eta}$ of eq. (1.18): From (2.11) and (2.9) one finds

$$\prod_i \lambda_i \;=\; \left(\frac{<\phi^{'} \mid \chi>}{<\phi^{'} \mid \phi>}\right)^{N-1} \;=\; \left(\frac{<\chi^{'} \mid \phi>}{<\phi^{'} \mid \phi>}\right)^{N-1} \;=\; \prod_i \lambda_i^{'} \;. \tag{2.12}$$

Furthermore

$$\overline{\eta}^{N-1} \;=\; \prod_i \lambda_i \;=\; \prod_i \lambda_i^{'} \;, \tag{2.13}$$

as is easily seen: Scalar multiplication of (2.7) by $<\varphi_i^{'} \mid$ and $\mid \varphi_i>$, respectively, gives together with (1.8) and (2.8):

$$\overline{\eta} \;=\; E \;-\; \frac{<\phi^{'} \mid H \mid \phi>}{<\phi^{'} \mid \phi>} \;=\; \eta_i \;-\; \frac{<\varphi_i^{'} \mid h \mid \varphi_i>}{<\varphi_i^{'} \mid \varphi_i>} \;=\; \lambda_i \, \frac{<\varphi_i^{'} \mid \chi_i>}{<\varphi_i^{'} \mid \varphi_i>} \;=\; \lambda_i^{'} \, \frac{<\chi_i^{'} \mid \varphi_i>}{<\varphi_i^{'} \mid \varphi_i>} \tag{2.14}$$

and with (2.11)

$$\overline{\eta} \;=\; \frac{<\phi^{'} \mid \chi>}{<\phi^{'} \mid \phi>} \;=\; \frac{<\chi^{'} \mid \phi>}{<\phi^{'} \mid \phi>} \;. \tag{2.15}$$

Combining (2.12) and (2.15) then results in (2.13).

It is now easy to obtain an equation for the density operator

$$\rho \;=\; \sum_{i=1}^{N} \frac{\mid \varphi_i><\varphi_i^{'} \mid}{<\varphi_i^{'} \mid \varphi_i>} \;, \tag{2.16}$$

using biorthogonality but leaving the normalization of the single–particle functions open. The dyadic product of (2.7) with $<\varphi_i^{'} \mid$ and $\mid \varphi_i>$ from right and left, respectively, gives

$$(\eta_i \,-\, h) \mid \varphi_i><\varphi_i^{'} \mid = \lambda_i \mid \chi_i><\varphi_i^{'} \mid \;\;;\;\; \mid \varphi_i><\varphi_i^{'} \mid (\eta_i \,-\, h) \,= \mid \varphi_i><\chi_i^{'} \mid \lambda_i^{'} \;. \tag{2.17}$$

Dividing by the norm $<\varphi_i^{'} \mid \varphi_i>$, summing over i and forming the difference finally results in:

$$[h, \rho] \;=\; \overline{\eta}\,(\rho_{\chi'} \,-\, \rho_{\chi}) \;, \tag{2.18}$$

if one defines the "mixed" densities

$$\rho_{\chi'} \;=\; \sum_{i=1}^{N} \frac{\mid \varphi_i><\chi_i^{'} \mid}{<\chi_i^{'} \mid \varphi_i>} \;\;;\;\; \rho_{\chi} \;=\; \sum_{i=1}^{N} \frac{\mid \chi_i><\varphi_i^{'} \mid}{<\varphi_i^{'} \mid \chi_i>} \tag{2.19}$$

and uses equation (2.14). This constitutes the proof of equation (1.18).

3 Path integral representation of the time–development operator

If a state χ is prepared at time t_i, then it will develop with time upto $t = t_f$ as

$$|\chi(t_f) >= U(t_f - t_i)|\chi > \tag{3.1}$$

with

$$U(t_f - t_i) = \exp\left\{-\frac{i}{\hbar}(t_f - t_i) H\right\} . \tag{3.2}$$

The probability of finding some state $|\chi' >$ at $t = t_f$ is then obtained from the amplitude

$$< \chi'|\chi(t_f) > = < \chi'|U(t_f - t_i)|\chi > . \tag{3.3}$$

An exact representation of the time–development operator of the many–body problem in terms of a time–dependent single–particle Hamiltonian can be achieved by the Hubbard–Stratonovich transformation. To this end one rewrites the full Hamiltonian H in terms of operators [3]

$$\rho_{\alpha\gamma} = a^\dagger_\alpha a_\gamma \tag{3.4}$$

in arbitrary orthonormal basis as

$$H = \sum_{\alpha,\gamma} K_{\alpha\gamma}\rho_{\alpha\gamma} + \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} \rho_{\alpha\gamma} v_{\alpha\beta\gamma\delta}\rho_{\beta\delta} \tag{3.5}$$

with matrix elements

$$v_{\alpha\beta\gamma\delta} = \int\int d^3\vec{r}\, d^3\vec{r}\,'\, \varphi^\star_\alpha(\vec{r})\varphi^\star_\beta(\vec{r}\,')\, v(\vec{r},\vec{r}\,')\, \varphi_\gamma(\vec{r})\varphi_\delta(\vec{r}\,') = (\alpha\beta|v|\gamma\delta) , \tag{3.6}$$

$$t_{\alpha\gamma} = \int d^3\vec{r}\,\varphi^\star_\alpha(\vec{r})\, t\, \varphi_\gamma(\vec{r}) \quad \text{and} \quad K_{\alpha\gamma} = t_{\alpha\gamma} - \frac{1}{2}\sum_\beta v_{\alpha\beta\beta\gamma}$$

in that basis. Whenever possible, we shall use the matrix notation

$$H = K\cdot\rho + \frac{1}{2}\rho\cdot v\cdot\rho \tag{3.7}$$

to avoid cumbersome labels and summations. The unphysical self–interaction term in (3.6), combined with the kinetic energy $t_{\alpha\gamma}$ into $K_{\alpha\gamma}$, arises from anticommuting creation and annihilation operators in the standard form of H such that the density operator representation (3.5) follows. We shall come back to this point in section 4. One then employs the Gaussian trick in its complex version,

$$\exp\left\{-\frac{i}{2}b\cdot A\cdot b\right\} = \sqrt{\det A^{-1}}\int\left(\prod_{j=1}^{L}\frac{dx_j}{\sqrt{2\pi i}}\right)\exp\left\{+\frac{i}{2}x\cdot A^{-1}\cdot x - ib\cdot x\right\} , \tag{3.8}$$

to the time development operator (3.2), identifying the density operator ρ with b. Relation (3.8) is valid if matrix A is real, symmetric and invertible.

The Gaussian trick (3.8) cannot be applied immediately to the two–body part of H in equation (3.5), since the one–body and two–body parts of H do not commute. This non–commutativity is treated the standard way by dividing the time–interval $(t_f - t_i)$ in (3.2) into M slices of equal length $\epsilon = (t_f - t_i)/M$. Then we can factorize for $\epsilon \to 0$,

$$\exp\left\{-\frac{i}{\hbar}\epsilon H\right\} = \exp\left\{-\frac{i}{\hbar}\epsilon K \cdot \rho\right\} \exp\left\{-\frac{i}{2\hbar}\epsilon \rho \cdot v \cdot \rho\right\} , \tag{3.9}$$

and we may now apply (3.8) to linearize the second factor of (3.9) in ρ:

$$\exp\left\{-\frac{i}{2\hbar}\epsilon \rho \cdot v \cdot \rho\right\} = \sqrt{\det\left(\frac{\epsilon}{\hbar} v^{-1}\right)} \int \left(\prod_{\alpha,\gamma} \frac{d\sigma_{\alpha\gamma}}{\sqrt{2\pi i}}\right) \exp\left\{\frac{i}{2\hbar}\epsilon \sigma \cdot v^{-1} \cdot \sigma - \frac{i}{\hbar}\epsilon \sigma \cdot \rho\right\} . \tag{3.10}$$

For each operator $\rho_{\alpha\gamma}$ we have to introduce a real variable $\sigma_{\alpha\gamma}$. Choosing

$$\tilde{\sigma} = \sigma \cdot v^{-1} , \tag{3.11}$$

we may also write

$$\exp\left\{-\frac{i}{2\hbar}\epsilon \rho \cdot v \cdot \rho\right\} = \sqrt{\det\left(\frac{\epsilon}{\hbar} v\right)} \int \left(\prod_{\alpha,\gamma} \frac{d\tilde{\sigma}_{\alpha\gamma}}{\sqrt{2\pi i}}\right) \exp\left\{\frac{i}{2\hbar}\epsilon \tilde{\sigma} \cdot v \cdot \tilde{\sigma} - \frac{i}{\hbar}\epsilon \tilde{\sigma} \cdot v \cdot \rho\right\} \tag{3.12}$$

as useful alternative to (3.10). While $\tilde{\sigma}$ has the quality of a density, σ has that of a potential. Matrix v of equation (3.6) is symmetric in particle coordinates $\vec{r}$, $\vec{r}'$ and thus in the label pairs (α, γ) and (β, δ). Hence v fulfills the symmetry requirement on A in formula (3.8).

Repeating the above step for each time–interval, labelled by index k in the following, we can write for the time–evolution operator (3.2) with (3.10):

$$\begin{aligned} \exp\left\{-\frac{i}{\hbar}(t_f - t_i) H\right\} &= \int \left(\prod_{k=1}^{M} \sqrt{\det\left(\frac{\epsilon}{\hbar} v^{-1}\right)} \prod_{\alpha,\gamma} \frac{d\sigma_{\alpha\gamma}(k)}{\sqrt{2\pi i}}\right) \\ &\times \exp\left\{\frac{i}{2\hbar}\epsilon \sum_{k=1}^{M} \sigma(k) \cdot v^{-1} \cdot \sigma(k)\right\} \prod_{k=1}^{M} \exp\left\{-\frac{i}{\hbar}\epsilon (K + \sigma(k)) \cdot \rho\right\} . \end{aligned} \tag{3.13}$$

To prepare the next step we note that from (3.10)

$$\left(\det\left(\frac{\epsilon}{\hbar} v^{-1}\right)\right)^{-\frac{1}{2}} = \int \left(\prod_{\alpha,\gamma} \frac{d\sigma_{\alpha\gamma}}{\sqrt{2\pi i}}\right) \exp\left\{\frac{i}{2\hbar}\epsilon \sigma \cdot v^{-1} \cdot \sigma\right\} . \tag{3.14}$$

We may now take the limit $\epsilon \to 0$, $M \to \infty$ such that $\epsilon M = (t_f - t_i)$ remains finite, replacing in (3.13)

$$\epsilon \sum_{k=1}^{M} \cdots \quad \longrightarrow \quad \int_{t_i}^{t_f} dt \cdots \quad . \tag{3.15}$$

Then (3.13) reads as functional integral, using the Trotter formula,

$$\begin{aligned} \exp\left\{-\frac{i}{\hbar}(t_f - t_i) H\right\} &= \frac{1}{\mathcal{N}} \int \left(\prod_{\alpha,\gamma} \frac{D\sigma_{\alpha\gamma}}{\sqrt{2\pi i}}\right) \\ &\times \exp\left\{\frac{i}{2\hbar}\int_{t_i}^{t_f} dt\, \sigma(t) \cdot v^{-1} \cdot \sigma(t)\right\} \mathcal{T}\left[\exp\left\{-\frac{i}{\hbar}\int_{t_i}^{t_f} dt\, (K + \sigma(t)) \cdot \rho\right\}\right] \end{aligned} \tag{3.16}$$

where $\mathcal{T}$ denotes time–ordering and the norm

$$\mathcal{N} = \int \left(\prod_{\alpha,\gamma} \frac{D\,\sigma_{\alpha\gamma}}{\sqrt{2\pi\, i}} \right) \exp \left\{ \frac{i}{2\,\hbar} \int_{t_i}^{t_f} dt\, \sigma\,(t) \cdot v^{-1} \cdot \sigma\,(t) \right\} \tag{3.17}$$

depends still on $T = t_f - t_i$, i.e. $\mathcal{N} = \mathcal{N}(T)$. As short–hand notation we shall use in the following

$$< \chi^{'}|U\,(T)|\chi >= \frac{1}{\mathcal{N}} \int D\sigma \exp \left\{ \frac{i}{2\,\hbar} \int\, dt\, \sigma\,(t) \cdot v^{-1} \cdot \sigma\,(t) \right\} < \chi^{'}|U_\sigma\,(T)|\chi > , \tag{3.18}$$

$$\mathcal{N} = \int\, D\sigma\, \exp \left\{ \frac{i}{2\,\hbar} \int\, dt\, \sigma\,(t) \cdot v^{-1} \cdot \sigma\,(t) \right\} ,$$

and

$$U_\sigma(T) = \mathcal{T}\, [\exp \left\{ - \frac{i}{\hbar} \int\, dt\, h_\sigma\,(t) \right\}]$$

with single–particle Hamiltonian

$$h\,(\sigma\,(t)) = h_\sigma\,(t) = (K + \sigma\,(t)) \cdot \rho\ . \tag{3.19}$$

The time–ordering operator $\mathcal{T}$ is necessary since in general

$$[h_\sigma(t),\, h_{\sigma^{'}}(t^{'})] \neq 0\ . \tag{3.20}$$

In (3.18) we have represented the time–evolution operator of a system with time–<u>independent</u> two–body interaction as superposition of time–evolution operators with time–<u>dependent</u> single–particle Hamiltonian $h_\sigma(t)$ defined through some collective field $\sigma(t)$. The superposition, being written as functional integral, contains the typical Gaussian weight factor in the field σ.

4 Ambiguities of the auxiliary field

There are two sources of ambiguity or, positively put, of freedom in the choice of the auxiliary field $\sigma\,(t)$ [3, 9]:

1. There are various ways to divide the Hamiltonian into one– and two–body parts,

$$H = T + V = (T + U) + (V - U) = H_0 + H^{'}\ , \tag{4.1}$$

a fact well–known from the static shell model. All such versions are equivalent in an exact treatment, however, approximate schemes of calculating physical quantities will obviously lead to different results.

With the choice (3.4) for the density operator ρ, the mean field σ, determined in lowest order of the stationary phase approximation to the functional integral (3.18), is of Hartree type. The Fock term appears only after quadratic corrections are taken into account. In contrast, choosing $\overline{\rho}_{\alpha\,\delta} = a_\alpha^\dagger\, a_\delta$ as density operator in (3.5), one obtains in lowest order the Fock–term only which in turn is corrected in second order by the Hartree–term. With $\Delta^\dagger_{\alpha\beta} = a^\dagger_\alpha a^\dagger_\beta$ and $\Delta_{\delta\gamma} = a_\gamma a_\delta$ it is possible to introduce pairing fields in lowest order.

All told, the solutions σ of the stationary phase approximation just define a starting point for higher orders of the stationary phase approximation. Their convergence rate will, of course, depend on the choice of the starting point.

2. The second ambiguity lies at the core of the functional integral representation introduced in section 3. In the expansion of the second term in the exponent of (3.12),

$$\exp\left\{-\frac{i}{\hbar}\epsilon\,\tilde{\sigma}\cdot v\cdot\rho\right\} = 1 - \frac{i}{\hbar}\epsilon\,\tilde{\sigma}\cdot v\cdot\rho - \frac{\epsilon^2}{2\hbar^2}(\tilde{\sigma}\cdot v\cdot\rho)^2\cdots\ , \tag{4.2}$$

the linear term does not contribute to the integral as it is odd. The contribution of (4.2) to the integral in (3.12) stems from the quadratic term in (4.2) which actually is of order ϵ, since with the Gaussian weight factor the dominant values of $\tilde{\sigma}$ are of order $\epsilon^{-\frac{1}{2}}$. We may, therefore, arbitrarily modify the coefficient of the term linear in $\tilde{\sigma}$ in (4.2), without changing the value of the integral (3.12). If we choose this coefficient as

$$W_{\alpha\beta\gamma\delta} = v_{\alpha\beta\gamma\delta} - v_{\alpha\beta\delta\gamma}\ , \tag{4.3}$$

then we will have included both Hartree and Fock terms already in lowest order stationary phase approximation (SPA).

This linear term is important when one determines the stationary value $\tilde{\sigma}^\circ$ of the integrand in (3.12), but does not contribute to the integral (3.12) or finally the functional integral in $\tilde{\sigma}$ corresponding to (3.18). Conversely the $\tilde{\sigma}$–quadratic terms in (4.2) do not influence the stationary value of $\tilde{\sigma}$, however, they must be taken into account when the functional integral over the fluctuations around $\tilde{\sigma}^\circ$ is calculated.

5 Stationary phase approximation

To evaluate the integrals in (3.18), we shall use the stationary phase approximation (SPA). We illustrate the method for a real, one–dimensional integral

$$I(l) = \int_{-\infty}^{\infty} dx\,\exp\left(-f(x)\,/\,l\right)\ . \tag{5.1}$$

For small l the integral is dominated by the stationary points of $f(x)$. If there is only one solution $f'(x_0) = 0$, then expansion of $f(x)$ upto second order in $(x - x_0)$ gives

$$\begin{aligned} I(l) &= \exp\left(-f(x_0)\,/\,l\right)\left\{\int_{-\infty}^{\infty} dx\,\exp\left(-\frac{(x-x_0)^2}{2\,l}f''(x_0)\pm\cdots\right)\right\} \\ &\approx \exp\left(-f(x_0)\,/\,l\right)\sqrt{\frac{2\pi l}{f''(x_0)}}\ , \end{aligned} \tag{5.2}$$

assuming a minimum ($f''(x_0) > 0$). The complex variant of (5.1), (5.2), extended to the multi–dimensional case, will be applied to the integral (3.18). The role of the small parameter l is then taken by $\hbar$. Hence the use of (5.2) implies a semi–classical expansion.

Rewriting (3.18) as

$$< \chi^{'}|U\,(T)|\chi > = \frac{1}{\mathcal{N}} \int D\sigma \, \exp \left\{ \frac{i}{\hbar} \, S\,[\sigma(t)] \right\} \tag{5.3}$$

with

$$S \; = \; \frac{1}{2} \int\limits_{t_i}^{t_f} dt \, \sigma\,(t) \; \cdot \; v^{-1} \; \cdot \; \sigma\,(t) \; - \; i\,\hbar \, \ln < \chi^{'}|\mathcal{T}\,[\exp(-\frac{i}{\hbar} \int\limits_{t_i}^{t_f} dt \, h_\sigma(t))]|\chi > \; , \tag{5.4}$$

the saddle point condition for the functional S,

$$\frac{\delta\, S}{\delta\, \sigma_{\alpha\gamma}(t)} \; = \; 0 \quad \text{for all} \quad \alpha, \, \gamma \; , \tag{5.5}$$

reads explicitly, in matrix notation,

$$\sigma^{\circ}\,(t) \; \cdot \; v^{-1} \; = \; \frac{< \chi^{'}|U_{\sigma^{\circ}}\,(t_f, \, t)\, \rho \, U_{\sigma^{\circ}}\,(t, \, t_i)|\chi >}{< \chi^{'}|U_{\sigma^{\circ}}\,(t_f, \, t_i)|\chi >} \tag{5.6}$$

with $U_{\sigma^{\circ}}\,(t'', \, t')$ the time–development operator under the single–particle Hamiltonian $h_{\sigma^{\circ}}\,(t)$. Note that σ° will in general be complex, although the σ–fields were originally introduced as real integration variables. If we take χ', χ as Slater determinants and generate χ' as

$$|\chi^{'} > = U_{\sigma^{\circ}}\,(t_f, \, t_i)|\chi > \; , \tag{5.7}$$

then (5.6) simplifies to the TDHF mean field

$$\sigma^{\circ}\,(t) \; = \; \frac{< \chi|U_{\sigma^{\circ}}\,(t_i, \, t)\, \rho \, U_{\sigma^{\circ}}\,(t, \, t_i)|\chi >}{< \chi|\chi >} \; \cdot \; v \tag{5.8}$$

which refers to the initial time t_i only.

The value of the functional integral (5.3) with action S from (5.4) is in lowest order

$$< \chi^{'}|U(T)|\chi > = \; \exp \left\{ \frac{i}{2\,\hbar} \int dt \, \sigma^{\circ}\,(t) \cdot v^{-1} \cdot \sigma^{\circ}\,(t) \right\} < \chi^{'}|U_{\sigma^{\circ}}(T)|\chi > \; . \tag{5.9}$$

The norm $\mathcal{N}(T)$ is canceled by the quadratic correction term corresponding to (5.2), if we ignore the second term in S, eq. (5.4). This term carries an $i\,\hbar$–factor which makes it weakly oscillating compared to the first term. This term, dropped in (5.9), generates the Fock term if one starts from the original version of equations (3.4) and (3.5) with Hartree term only, and it cancels the self–interaction term in (3.6). It also reproduces correlations of the random phase approximation [3].

Taking χ, χ' as Slater determinants, the equation of motion for the density operator is obtained from (3.18), (3.19) and (5.6) by defining Slater determinants

$$|\Psi\,(t) > = \; U_{\sigma^{\circ}}(t, \, t_i)|\chi > \quad ; \quad < \tilde{\Psi}(t)| \; = < \chi^{'}|U_{\sigma^{\circ}}\,(t_f, \, t) \; . \tag{5.10}$$

The time dependence of the respective single–particle functions $\psi_i(t)$, $\tilde{\psi}_i(t)$ is then governed by

$$i\,\hbar\,\frac{\partial}{\partial t}\,|\,\psi_i(t)> = h_{\sigma^\circ}(t)|\psi_i(t)> \quad ; \quad -i\,\hbar\,\frac{\partial}{\partial t} < \tilde{\psi}_i(t)| = < \tilde{\psi}_i(t)|h_{\sigma^\circ}(t) \tag{5.11}$$

with time boundary conditions

$$\psi_i(t_i) = \chi_i \; ; \; \tilde{\psi}_i(t_f) = \chi_i' \quad . \tag{5.12}$$

For the density operator

$$\rho = \sum_{i=1}^{N} \frac{|\,\psi_i(t) >< \tilde{\psi}_i(t)\,|}{< \tilde{\psi}_i(t)|\psi_i(t) >} \tag{5.13}$$

one then immediately confirms eq. (1.7),

$$i\,\hbar\,\frac{\partial}{\partial t}\,\rho = [h_{\sigma^\circ}(t), \rho] \; . \tag{5.14}$$

Equation (5.14) has to be solved under time–boundary conditions, at $t = t_i$ and t_f, rather than as initial value problem like (1.1), (1.2). Each transition $\chi \to \chi'$ will have its own mean field, and this allows the method to describe exclusive reactions in contrast to TDHF which at best can be used for inclusive reactions. It is also worth noting that TDMF needs two sets of single–particle wave functions, $\psi_i(t)$ and $\tilde{\psi}_i(t)$, while TDHF is formulated in just one set which develops from the initial state in the mean field u.

6 Static approximation

On the exact many–body level the connection between the resolvent and the time–development operator is simply a Fourier transformation

$$< \chi'|(E + i\,\kappa - H)^{-1}|\chi > = -\frac{i}{\hbar}\int_0^\infty dT\,\exp\left\{\frac{i}{\hbar}(E + i\,\kappa)\,T\right\} < \chi'|\exp\left(-\frac{i}{\hbar}\,H\,T\right)|\chi > \tag{6.1}$$

for infinitesimal $\kappa > 0$ and with χ, χ' as initial and final states. On the mean field level the connection between the resolvent and time–development operator is more intricate due to the non–linear nature of self–consistent mean field methods.

The basic assumption to be made is that $\sigma(t)$ and hence $h_\sigma(t)$ vary slowly in time so that we may approximately neglect their time dependence. In this static approximation we have from (3.18) and (3.19)

$$< \chi'|\exp\left\{-\frac{i}{\hbar}\,H\,T\right\}|\chi > = \frac{1}{\mathcal{N}(T)}\int D\sigma\,\exp\left\{\frac{i}{2\hbar}(\sigma\cdot v^{-1}\cdot\sigma)\,T\right\} < \chi'|\exp\left\{-\frac{i}{\hbar}\,h_\sigma\,T\right\}|\chi > \tag{6.2}$$

so that (6.1) reads:

$$< \chi'|(E + i\,\kappa - H)^{-1}|\chi > = \tag{6.3}$$

$$-\frac{i}{\hbar}\int_0^\infty dT \exp\left\{\frac{i}{\hbar}(E+i\kappa)T\right\}\frac{1}{\mathcal{N}(T)}\int D\sigma \exp\left\{\frac{i}{2\hbar}(\sigma\cdot v^{-1}\cdot\sigma)T\right\} < \chi^{'}|\exp\left\{-\frac{i}{\hbar}h_\sigma T\right\}|\chi > \quad .$$

In N–particle Hilbert space with

$$h_\sigma \;=\; \sum_{m\,=\,1}^{N} h_m\,(\sigma)\;, \tag{6.4}$$

we can use the inverse Fourier transformation on the single–particle level,

$$\exp\left\{-\frac{i}{\hbar}(h_m \,-\, i\,\kappa_m)\,T\right\} \;=\; \frac{i}{2\pi}\int_{-\infty}^{\infty} dw_m\;\frac{\exp\left\{-\frac{i}{\hbar}\,w_m\,T\right\}}{w_m\,-\,h_m\,+\,i\,\kappa_m} \quad \text{with} \quad T\,>\,0 \tag{6.5}$$

for particle m, to obtain an expression for the many–body resolvent in terms of single–particle resolvents $g_m = (w_m - h_m + i\kappa_m)^{-1}$

$$< \chi^{'}|(E\,+\,i\,\kappa\,-\,H)^{-1}|\chi> = -\frac{i}{\hbar}\left(\frac{i}{2\pi}\right)^N\int_0^\infty dT\frac{1}{\mathcal{N}(T)}\int D\sigma\int\left(\prod_{m=1}^{N}\,dw_m\right) \tag{6.6}$$

$$\times\;\exp\left\{\frac{i}{\hbar}(E+i\kappa^{'}-\sum_m w_m+\frac{1}{2}\sigma\cdot v^{-1}\cdot\sigma)T\right\} < \chi^{'}|\prod_{m\,=\,1}^{N}(w_m\,-\,h_m\,+\,i\,\kappa_m)^{-1}|\chi>$$

with the constraint $\kappa^{'} = \kappa - \sum_m \kappa_m > 0$ to ensure the existence of the T–integral.

The product of single–particle operators in (6.6) acting on the Slater determinant χ (to the right or on $\chi^{'}$ to the left) gives

$$\left(\prod_{m\,=\,1}^{N} g_m\right)\;\mathcal{A}|\chi_1\,\chi_2\ldots\chi_N> = \;\mathcal{A}|(g_1\,\chi_1)\,(g_2\,\chi_2)\ldots(g_N\,\chi_N)> \tag{6.7}$$

since the antisymmetrizer $\mathcal{A}$ commutes with the symmetrical product $\prod_m g_m$. Equation (6.7) suggests to introduce two sets of single–particle wave functions

$$|\;\varphi_m> = \;g_m\;|\;\chi_m>\;\;;\;\;<\varphi^{'}_m\;| = <\chi^{'}_m\;|\;g_m \tag{6.8}$$

or equivalently

$$(w_m\,-\,h)\;|\;\varphi_m\,(\sigma,\,w_m)> = |\;\chi_m>\;\;;\;\;<\varphi^{'}_m\,(\sigma,\,w_m)\;|\;(w_m\,-\,h)\;=<\chi^{'}_m\;|\;\;. \tag{6.9}$$

Note that on the single–particle level we may now drop the label m on the Hamiltonian h being the same for all (identical!) particles. In this representation

$$<\chi^{'}|(E+i\kappa-H)^{-1}|\chi> = -\frac{i}{\hbar}\left(\frac{i}{2\,\pi}\right)^N\int_0^\infty dT\int D\sigma\int\left(\prod_m dw_m\right)\frac{1}{\mathcal{N}(T)}\exp\left\{\frac{i}{\hbar}S\,[\sigma,\,w_m,\,T]\right\} \tag{6.10}$$

with

$$S\;=\;\left(E\,+\,i\,\kappa^{'}\,+\,\frac{1}{2}\sigma\,\cdot\,v^{-1}\,\cdot\,\sigma\,-\,\sum_m\,w_m\right)\;T\;-\;i\,\hbar\,\sum_m\,\ln<\chi^{'}_m\;|\;\varphi_m>\;\;. \tag{6.11}$$

In the last term in (6.11) we can replace $< \chi'_m \mid \varphi_m >$ by $< \varphi'_m \mid \chi_m >$ using the bra– rather than the ket–equation in (6.8). In both versions we assume, with the same arguments as in section 2, that the overlap matrices $< \chi'_m \mid \varphi_n >$ and $< \varphi'_m \mid \chi_n >$ are chosen diagonal. Eqs. (6.5) and (6.8), (6.9) establish a Fourier transformation on the single–particle level between $\psi_m(T)$ and $\varphi_m(w_m)$:

$$\begin{aligned} |\psi_m(T)> &= \exp\left\{-\frac{i}{\hbar}(h - i\,\kappa_m)\,T\right\} |\chi_m> \\ &= \frac{i}{2\pi}\int_{-\infty}^{\infty} d\,w_m \frac{\exp\left\{-\frac{i}{\hbar}\,w_m\,T\right\}}{w_m - h - i\,\kappa_m} |\chi_m> \\ &= \frac{i}{2\,\pi}\int_{-\infty}^{\infty} d\,w_m \exp\left\{-\frac{i}{\hbar}\,w_m\,T\right\} |\varphi_m(w_m)> \quad . \end{aligned} \tag{6.12}$$

Equations (6.9) have, apart from the normalization factors λ_i, λ'_i, the formal structure of (2.7). However, energies w_m were introduced as real variables in contrast to the complex η_i of (2.7), and h in (6.9) is defined in terms of the σ–fields rather than through φ_m, φ'_m. Only after we have solved all integrations of (6.10) in SPA, we will recover the inhomogeneous TIMF equations (2.7) together with the correct value of the resolvent matrix element (2.9).

7 Path and energy integrals

These integrals will be solved simultaneously in SPA, followed by the T–integration. While the energies w_m and auxiliary fields $\sigma_{\alpha\gamma}$ are introduced as real, independent variables, their stationary values will be complex and coupled through self–consistency.

The stationarity equations with respect to σ and w_m read:

$$\frac{\delta\,S}{\delta\,\sigma} = T\,\sigma\cdot v^{-1} - i\,\hbar\sum_{m=1}^{N}\frac{< \chi'_m \mid \frac{\delta}{\delta\,\sigma} \mid \varphi_m >}{< \chi'_m \mid \varphi_m >} = 0 \tag{7.1}$$

$$\frac{\partial\,S}{\partial\,w_n} = -T - i\,\hbar\sum_{m=1}^{N}\frac{< \chi'_m \mid \frac{\partial}{\partial\,w_n} \mid \varphi_m >}{< \chi'_m \mid \varphi_m >} = 0\ . \tag{7.2}$$

The above derivatives of φ_m can be calculated with the help of equations (6.9): Multiplying

$$(w_m - h)\,\frac{\delta}{\delta\,\sigma} \mid \varphi_m > - \frac{\delta\,h}{\delta\,\sigma} \mid \varphi_m >= 0 \tag{7.3}$$

by $< \varphi'_m \mid$ gives, with h from (3.19),

$$< \chi'_m \mid \frac{\delta}{\delta\,\sigma} \mid \varphi_m >=< \varphi'_m \mid \rho \mid \varphi_m > \quad . \tag{7.4}$$

Explicitly:

$$< \chi'_m \mid \frac{\delta}{\delta\,\sigma_{\alpha\gamma}} \mid \varphi_m >=< \varphi'_m \mid a^\dagger_\alpha\,a_\gamma \mid \varphi_m >=< \varphi'_m \mid \alpha >< \gamma \mid \varphi_m > \quad . \tag{7.5}$$

Derivatives of (6.9) with respect to w_n give

$$\delta_{nm} \left\{ \mid \varphi_m > + (w_m - h) \frac{\partial}{\partial w_n} \mid \varphi_m > \right\} = 0 \ . \tag{7.6}$$

Multiplying by $< \varphi_m' \mid$ and using again (6.9) leads to

$$< \chi_m' \mid \frac{\partial}{\partial w_n} \mid \varphi_m > = - \delta_{m\,n} < \varphi_m' \mid \varphi_m > \ . \tag{7.7}$$

We insert relations (7.4) and (7.7) into (7.1) and (7.2) to find the explicit stationarity equations. The stationary value of σ is given by

$$\sigma^\circ \cdot v^{-1} = \frac{i\hbar}{T} \sum_m \frac{< \varphi_m' \mid \rho \mid \varphi_m >}{< \chi_m' \mid \varphi_m >} \tag{7.8}$$

or

$$\sigma^\circ = \frac{i\hbar}{T} \sum_m \frac{< \varphi_m' \mid \rho \mid \varphi_m > \cdot v}{< \chi_m' \mid \varphi_m >} \ . \tag{7.9}$$

Explicitly with labels of single–particle states

$$\sigma^\circ_{\alpha\gamma} = \frac{i\hbar}{T} \sum_{\substack{m \\ \beta,\,\delta}} \frac{< \varphi_m' \mid \beta >< \delta \mid \varphi_m >}{< \chi_m' \mid \varphi_m >} v_{\beta\,\alpha\,\delta\,\gamma} = \frac{i\hbar}{T} \sum_m \frac{< \varphi_m' \,\alpha \mid v \mid \varphi_m \,\gamma >}{< \chi_m' \mid \varphi_m >} \tag{7.10}$$

using the completeness of single–particle states β, δ referring to the representation (3.5) of the Hamiltonian H. The stationary value w°_m is determined implicitly through

$$\frac{< \varphi_m' \mid \varphi_m >}{< \chi_m' \mid \varphi_m >} = - \frac{i}{\hbar} T \tag{7.11}$$

or, using (6.9) again, explicitly by

$$\frac{i\hbar}{T} = \frac{< \chi_m' \mid \varphi_m >}{< \varphi_m' \mid \varphi_m >} = \frac{< \varphi_m' \mid (w^\circ_m - h) \mid \varphi_m >}{< \varphi_m' \mid \varphi_m >} = w^\circ_m - \varepsilon^\circ_m \tag{7.12}$$

with

$$\varepsilon^\circ_m = \frac{< \varphi_m' \mid h(\sigma^\circ) \mid \varphi_m >}{< \varphi_m' \mid \varphi_m >} \ . \tag{7.13}$$

After T–integration in section 8, E rather than T^{-1} will appear in relation (7.12). Combining (7.10) and (7.11) identifies σ° as <u>Hartree–Fock</u> field,

$$\sigma^\circ_{\alpha\gamma} = \sum_{m=1}^{N} \frac{< \varphi_m' \,\alpha \mid v \mid \varphi_m \,\gamma >}{< \varphi_m' \mid \varphi_m >} \ , \tag{7.14}$$

since according to section 4 the matrix v is assumed to be antisymmetrized. A slight modification of (4.3) also allows to eliminate the unphysical self interaction in (3.6) so that K reduces to the kinetic energy operator.

The normalization factors in (6.10), $\mathcal{N}(T)$ and $(i\,/\,2\,\pi)^N$, are eliminated by the Gauss correction to the lowest order SPA which approximates the integrals by the integrand taken at the stationary point $(\sigma^\circ,\, w^\circ)$. The Gauss correction to the σ–integral,

$$\left(\det\left(\frac{\delta^2\,S}{\delta\sigma\,\delta\sigma'}\right)_{\sigma^\circ}\right)^{-\frac{1}{2}} = \left(\det\,(T\,v^{-1})\right)^{-\frac{1}{2}} \quad , \tag{7.15}$$

cancels $\mathcal{N}(T)$ according to (3.14), if the σ–dependence of the ln–term in (6.11) is neglected. This ln–term carries a factor $\hbar$ as compared to the leading term. Hence the above assumption is justified in semi–classical approximation. For the Gauss correction to the w–integration, each integral can be treated separately as the integrand factorizes. From (7.2) and (7.7), together with (6.9) and (7.12), it follows that the leading term in the second derivative of S with respect to w_m is given by

$$\left(\frac{\partial^2\,S}{\partial\,w_m^2}\right)_{w_m^\circ} = \frac{i}{\hbar}\,T^2 \quad , \tag{7.16}$$

and the total correction factor is

$$\sqrt{\prod_m\left(\frac{2\,\pi\,i\,\hbar}{S''(w_m)}\right)_{w_m^\circ}} = \left(\sqrt{2\,\pi}\;\frac{\hbar}{T}\right)^N \quad . \tag{7.17}$$

The correction to (7.16) involves fluctuations of the single–particle propagators which go beyond the mean field concept.

To this order the matrix element (6.10) of the resolvent reads

$$D\,(E\,+\,i\,\kappa) \;=\; <\chi^{'}|(E\,+\,i\,\kappa\,-\,H)^{-1}|\chi> \;= \tag{7.18}$$

$$-\frac{i}{\hbar}\left(\frac{e}{\sqrt{2\pi}}\right)^N\int\limits_0^\infty dT\left(\frac{i\hbar}{T}\right)^N\exp\left\{\frac{i}{\hbar}\left(E+\frac{1}{2}\,\sigma^\circ\cdot v^{-1}\cdot\sigma^\circ-\sum_m\varepsilon_m^\circ+i\kappa^{'}\right)T\right\} < \chi^{'}\mid\phi> \,,$$

after replacing w_m° by ε_m° according to (7.12). With $e\,/\sqrt{2\,\pi} = 1.084...$, the normalization factor $(i\,/\,2\,\pi)$ is not exactly cancelled by the Gaussian correction. However, this is just a constant, real factor which does not harm the analytical properties of the resolvent.

8 T–integration

With regard to SPA, we extend the range of integration for T to $-\infty$, introducing the step function in its integral representation,

$$\Theta\,(T) \;=\; \frac{1}{2\,\pi\,i}\int\limits_{-\infty}^{\infty} ds\,\frac{e^{\frac{i}{\hbar}\,s\,T}}{s\,-\,i\,\kappa''} \quad \text{for}\;\; \kappa'' > 0\;. \tag{8.1}$$

Then, with $e\,/\sqrt{2\,\pi}\approx 1$, we have

$$D\,(E\,+\,i\,\kappa) \;=\; \frac{1}{2\,\pi\,\hbar}\int\limits_{-\infty}^{\infty} dT\int\limits_{-\infty}^{\infty} ds\,\exp\left\{\frac{i}{\hbar}\,S[s,\,T]\right\} \tag{8.2}$$

with

$$S\,[s,\,T] \;=\; \left(E \,+\, \frac{1}{2}\,\sigma^\circ \,\cdot\, v^{-1} \,\cdot\, \sigma^\circ \,-\, \sum_m \varepsilon^\circ_m \,+\, s \,+\, i\,\kappa^{'}\right)\,T$$

$$-\,i\,\hbar\,\sum_m \ln < \chi^{'}_m \mid \varphi_m > \,-\,i\,\hbar\,N\,\ln\left(\frac{i\,\hbar}{T}\right) \,+\, i\,\hbar\,\ln\,(-s \,+\, i\,\kappa^{''})\;. \tag{8.3}$$

Simultaneous SPA to both integrals gives as stationarity equations

$$\frac{\partial\,S}{\partial\,s} \;=\; T \,+\, \frac{i\,\hbar}{s \,-\, i\,\kappa^{''}} \;=\; 0 \quad \text{or} \quad -\,s_\circ \;=\; \frac{i\,\hbar}{T_\circ} \tag{8.4}$$

and

$$\frac{\partial\,S}{\partial\,T} \;=\; E \,+\, \frac{1}{2}\,\sigma^\circ \,\cdot\, v^{-1} \,\cdot\, \sigma^\circ \,-\, \sum_m \varepsilon^\circ_m \,+\, s \,+\, i\,\kappa^{'} \;=\; 0 \tag{8.5}$$

$$\text{or} \quad -\,s_\circ \;=\; E \,+\, \frac{1}{2}\,\sigma^\circ \,\cdot\, v^{-1} \,\cdot\, \sigma^\circ \,-\, \sum_m \varepsilon^\circ_m$$

where $\kappa^{'}$, $\kappa^{''}$ are now superfluous. Eq. (8.5) is <u>exact</u> though it looks as if in (8.3) only the term proportional to T had been taken into account. The contributions from the remaining terms cancel exactly by virtue of eqs. (6.9).

For the Gauss correction to the lowest order SPA of the T– and s–integrals, one has to calculate the Hesse–matrix M of S with respect to T and s since S is not additive in the variables T and s. One finds

$$M \;=\; \begin{pmatrix} 0 & 1 \\ 1 & \frac{i}{\hbar}\,T_\circ^2 \end{pmatrix} \tag{8.6}$$

with

$$\frac{\partial^2\,S}{\partial\,T^2} \;=\; 0 \tag{8.7}$$

in semi–classical approximation. Hence $\det M = -1$, and the Gauss correction factor for the T– and s–integrations is $\sqrt{-(2\pi\hbar i)^2} = 2\pi\hbar$, which cancels the corresponding factor in (8.2). To this order of SPA we have

$$\begin{aligned} D\,(E \,+\, i\,\kappa) \;&=\; \exp\left\{\frac{i}{\hbar}\,S\,[T_\circ,\,s_\circ]\right\} \;=\; \left(\frac{i\,\hbar}{T_\circ}\right)^{N-1} < \chi^{'}|\phi > \\ &=\; \left(E \,+\, \frac{1}{2}\,\sigma^\circ \,\cdot\, v^{-1} \,\cdot\, \sigma^\circ \,-\, \sum_m \varepsilon^\circ_m\right)^{N-1} < \chi^{'}|\phi >\,, \end{aligned} \tag{8.8}$$

with $\phi = \phi(\sigma^\circ, w^\circ_m)$. The same result is obtained following an alternative line of reasoning: In the above semi–classical approximation, with S linear in T and derivative $\partial\,S\,/\,\partial\,T \;=\; E + \frac{1}{2}\sigma^\circ \cdot v^{-1} \cdot \sigma^\circ - \sum\limits_m \varepsilon^\circ_m + s$ independent of T, the T–integral reduces to a δ–distribution,

$$\frac{1}{2\pi\hbar}\int\limits_{-\infty}^{\infty} dT \exp\left\{\frac{i}{\hbar}\left(E + \frac{1}{2}\sigma^\circ \cdot v^{-1} \cdot \sigma^\circ - \sum_m \varepsilon^\circ_m + s\right)T\right\} = \delta\left(E + \frac{1}{2}\sigma^\circ \cdot v^{-1} \cdot \sigma^\circ - \sum_m \varepsilon^\circ_m + s\right). \tag{8.9}$$

With $(i\hbar/T)$ from the stationarity condition (8.4), the remaining s–integral can then be solved exactly,

$$\int\limits_{-\infty}^{\infty} d\,s \, \frac{\delta\left(E + \frac{1}{2}\sigma^\circ \cdot v^{-1} \cdot \sigma^\circ - \sum\limits_m \varepsilon_m^\circ + s\right)}{-\,s} (-\,s)^N < \chi^{'}|\phi> = (-\,s_\circ)^{N-1} < \chi^{'}|\phi> \quad (8.10)$$

with $s_\circ$ from (8.5), in complete agreement with (8.8).

9 Conclusions

With σ° from stationarity condition (7.14), the single–particle Hamiltonian $h\,(\sigma^\circ)$, eq. (3.19), has precisely the structure of h of section 2 with expectation value

$$\varepsilon_m^\circ = \frac{<\varphi_m^{'} \mid (t + \sigma^\circ) \mid \varphi_m>}{<\varphi_m^{'} \mid \varphi_m>} = \frac{<\varphi_m^{'} \mid (t + u) \mid \varphi_m>}{<\varphi_m^{'} \mid \varphi_m>} \,. \quad (9.1)$$

From (7.8), (7.11) and (7.14) one finds

$$\frac{1}{2}\sigma^\circ \cdot v^{-1} \cdot \sigma^\circ = \frac{1}{2}\sum_m \frac{<\varphi_m^{'} \mid \sigma^\circ \mid \varphi_m>}{<\varphi_m^{'} \mid \varphi_m>} = \frac{1}{2}\sum_{m,n} \frac{<\varphi_m^{'}\,\varphi_n^{'} \mid v \mid \varphi_m\,\varphi_n>}{<\varphi_m^{'} \mid \varphi_m><\varphi_n^{'} \mid \varphi_n>} \quad (9.2)$$

so that with (7.12), (8.4) and (8.5)

$$E + \frac{1}{2}\sigma^\circ \cdot v^{-1} \cdot \sigma^\circ - \sum_m \varepsilon_m^\circ = E - \frac{<\phi^{'} \mid H \mid \phi>}{<\phi^{'} \mid \phi>} = \overline{\eta} = w_m^\circ - \varepsilon_m^\circ = \frac{i\,\hbar}{T_\circ} \,, \quad (9.3)$$

and we can identify the (complex) stationary value w_m° with η_m of eq. (2.8). Hence eqs. (6.9) and (2.7) differ only by factors λ_i, $\lambda_i^{'}$ and we have to identify

$$\varphi_m\,(\sigma^\circ,\, w_m^\circ) = \frac{\varphi_m}{\lambda_m} \;\; ; \;\; \varphi_m^{'}\,(\sigma^\circ,\, w_m^\circ) = \frac{\varphi_m^{'}}{\lambda_m^{'}} \,. \quad (9.4)$$

We make now use of (2.13) to obtain the final result for (8.8)

$$D\,(E + i\,\kappa) = < \chi^{'}|\phi> = < \phi^{'}|\chi> \quad (9.5)$$

which fully agrees with equation (2.9) for the stationary value of functional F in the TIMF–method. In summary we can state that we have derived the inhomogeneous single–particle equations <u>and</u> the stationary value of the Green function of the TIMF–method from the TDMF in static, semi–classical approximation, with the Gauss–correction to the lowest order SPA taken into account.

Under various conceptual and practical criteria, TIMF can be placed between TDMF and TDHF (see also table 1): Both TDMF and TIMF methods calculate a mean field for each transition $\chi \to \chi^{'}$. Hence the respective transition amplitudes and resolvent matrix elements refer to exclusive reactions, while TDHF is applicable to inclusive reactions only. TDMF is conceptually superior to TIMF, the latter being a static approximation of the former method. Alternately put, TIMF is "local" in energy whereas TDMF is "non–local" in time. From the practical point of view, TIMF requires solving inhomogeneous, complex equations of Hartree–Fock type for given energy. In this respect it is comparable to TDHF which is "local" in time. The problem of TDMF lies in combining self–consistency with given boundary conditions in time. No practicable algorithm for this highly "non–local" problem seems to exist for use in actual numerical calculations. The practical advantage of TIMF becomes even more pronounced when considering the S–matrix. TDMF then has to calculate three auxiliary fields rather than one [2, 3] while the corresponding T–matrix of TIMF [6, 7] is obtained again from inhomogeneous, complex equations of Hartree–Fock type as for the above resolvent, with only slight generalization of the inhomogeneities.

Acknowledgements:
One of us (A.W.) wants to thank the Japan Society for Promotion of Science and the Deutsche Akademische Austauschdienst for financial support during his stay in Japan. He is also very grateful for the hospitality found at the Yukawa Institute for Theoretical Physics in Kyoto and for helpful discussions with Y. Abe and H. Horiuchi.

References:

1. K. Goeke, R. Y. Cusson, F. Grümmer, P.-G. Reinhard and H. Reinhardt: Prog. Theor. Phys. [Suppl.] **74 & 75**, 33 (1983)
2. H. Reinhardt: Nuclear Physics A **390**, 70 (1982)
3. J. W. Negele and H. Orland: Quantum Many–Particle Systems (Addison–Wesley, 1988)
4. H. Reinhardt: Fortschr. d. Physik **30**, 127 (1982)
5. J. P. Blaizot and G. Ripka: Quantum Theory of Finite Systems (MIT Press, 1986)
6. B. Giraud, M. A. Nagarajan and I. J. Thompson, Ann. Phys. (N. Y.) **152**, 475 (1984); B. Giraud, M. A. Nagarajan, Ann. Phys. (N. Y.) **212**, 260 (1991)
7. J. C. Lemm, Ann. Phys. (N. Y.) **244**, 136 (1995)
8. A. Wierling, B. Giraud, F. Mekideche, H. Horiuchi, T. Maruyama, A. Ohnishi, J. C. Lemm and A. Weiguny, Z. Phy. A **348**, 153 (1994)
9. A. K. Kerman, S. Levit and T. Troudet: Ann. Phys. (N. Y.) **148**, 436 (1983)

Mean Field Methods for Reactions

Time–Dependent | Time–Independent

Basic quantity

$$< \chi' \mid \exp\{-\tfrac{i}{\hbar}(t_f - t_i)H\} \mid \chi > \quad \overset{\text{Fourier}}{\underset{\text{Transformation}}{\Longleftrightarrow}} \quad < \chi' \mid (E - H)^{-1} \mid \chi >$$

$$\Downarrow \qquad\qquad\qquad\qquad \Downarrow$$

Mean Field Approximation

$$\text{TDHF} \quad \overset{\text{restriction of } \chi'}{\underset{|\chi'>=U_h(t_f-t_i)|\chi>}{\Longleftarrow}} \quad \text{TDMF} \quad \overset{\text{static}}{\underset{\text{approximation}}{\Longrightarrow}} \quad \text{TIMF}$$

	TDHF	TDMF	TIMF
Equation of motion	$[h, \rho] = i\hbar\dot{\rho}$	$[h, \rho] = i\hbar\dot{\rho}$	$[h, \rho] = \overline{\eta}(\rho_{\chi'} - \rho_{\chi})$
	to be solved for given		
	$\rho(t_i)$	$\rho(t_i)\,,\ \rho(t_f)$	$\chi\,,\ \chi'$
Type of problem	initial	boundary	inhomogeneous problem
	condition problem in t:		parametric in E:
	"local"	"non–local"	"local"
Representation of density ρ in basis	$\mid \psi_m(t) >$	$\mid \psi_m(t) >\,,\ < \tilde{\psi}_m(t) \mid$	$\mid \varphi_m >\,,\ < \varphi'_m \mid$
	orthogonal	biorthogonal	biorthogonal
Single–particle Hamiltonian h	Hermitian	non–Hermitian	non–Hermitian
Specification of asymptotic channels	no	yes	yes
Reactions described	inclusive	exclusive	exclusive

Table 1