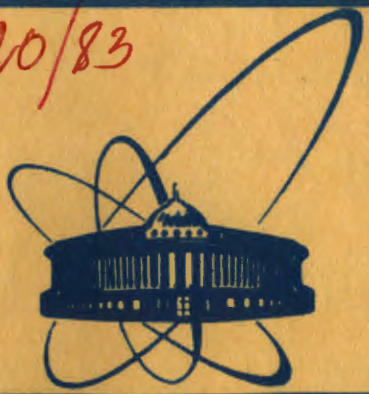

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SHORT-RANGE CORRELATIONS IN AN EXTENDED TIME-DEPENDENT MEAN-FIELD THEORY

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1. Introduction

Over the last years a large number of investigations have demonstrated the effectiveness of the time-dependent Hartree-Fock (TDHF) approximation[1] as a theory of large amplitude nuclear dynamics (see for example refs.[2-4] and literature cited therein).

Besides the classical (deterministic) character of the TDHF initial value problem the emission of the two-body correlations caused by the residual interaction is one of the main disadvantages of the theory. Furthermore, ordinary TDHF as well as such extended mean-field theories cannot deal with realistic nucleon-nucleon forces due to the strong repulsion between the particles at short distances. To avoid diverging matrix elements and to consistently resum certain higher order terms of the full many-body problem the bare interaction is replaced by an effective interaction commonly taken in the phenomenological Skyrme form[2-4].

Our aim is to propose an extension of TDHF which, in some approximation to be discussed below, includes two-body correlations on a level of microscopic reversibility relating them to realistic nucleon--nucleon forces. Because we are not able to realize such a program with respect to the full range of the two-body potential we restrict ourselves to the consideration of strong short-range components of the potential on a level of correlations only between nearest neighbours. We consider higher order effects as well as long-range correlations only to the extent to which they contribute to the mean field which, of course, is not the same as in TDHF because of the explicit description of short-range correlations (SRC) in lowest order.

The mean-field theory itself relies on the statement that up to a certain energy, e.g., in a heavy ion reaction, the Pauli exlusion principle effectively suppresses LRC's. On the other hand SRC's being connected with very large momentum transfers up to several Fermi momenta are not influenced by the Pauli principle at all and essentially contribute even to the nuclear ground state energy (for a recent example see ref.[5]). Such high-lying components in the nucleonic momentum distribution cannot be reproduced by any determinantal wave function[6].

Therefore, it seems to be an interesting task to include SRC's from the outset and to look for its dynamical realizations in the framework of the proposed picture.

In the present paper we outline an extension of the mean-field theory starting from the method of correlated basis functions (CBF) /7-9/, which provides a natural framework for the description of strongly interacting Fermi systems. A more detailed version of this work is given in ref. /10/. In sect. 2 we derive the extended mean-field equations. Sect. 3 deals with the corresponding correlated stationary problem and the choice of appropriate initial conditions. The one-body density matrix of the correlated system is evaluated in sect. 4.

2. Extended Mean-Field Equations

We start with the choice of time-dependent many-particle trial wave functions as

$$\Psi(1\ldots A,t) = C^{-\frac{1}{2}}\, F\, \mathcal{A} \prod_{i=1}^{A} \phi_i(i,t) \qquad (2.1)$$

with $C = \langle\Psi|\Psi\rangle$ and $\mathcal{A}$ being the A-particle antisymmetrizer. F is a symmetric, translationally invariant correlation operator having the cluster decomposition property /7/. The single-particle model states ϕ_i are required to reflect properly the long-range order of the nuclear system while F has the task of incorporating the most essential dynamical correlations, the short-range correlations in our case. The choice of a single determinantal configuration in eq. (2.1) does not exhaust the full power of the CBF method /7/ but reflects our approximation that LRC's are considered only via the mean field.

The time-dependent operator F is chosen in the form

$$F = \prod_{1\le i<j\le A} F(i,j,t) \quad , \quad F(i,j,t) = \sum_l f_l(r_{ij},t)\, P_l \qquad (2.2)$$

according to a local central symmetric two-body potential

$$V(i,j) = \sum_l V_l(r_{ij})\, P_l \qquad (2.3)$$

with P_l being the projector onto the l-th partial wave of relative motion of nucleons i and j at distance r_{ij}. The real, non-negative correlation functions $f_l(r)$ are to be small (or zero) inside the small-r core region and approach unity at large r.

We rewrite the nuclear Hamiltonian identically as

$$H = \sum_i t(i) + \sum_{i<j} V(i,j) \equiv \sum_i H_1(i,t) + \sum_{i<j} V_{res}(i,j,t) \qquad (2.4)$$

introducing an arbitrary time-dependent one-body potential $U(i,t)$ and a time-dependent residual interaction $V_{res}(i,j,t)$ as

$$H_1(i,t) = t(i) + U(i,t) \qquad (2.5)$$

$$V_{res}(i,j,t) = V(i,j) - \frac{1}{(A-1)}\left[U(i,t) + U(j,t)\right] \quad . \qquad (2.6)$$

In general, if choosing an unreasonable form of the potential U, the residual interaction defined by eq. (2.6) is of very long range. We wish, however, to realize our approximation to include LRC's only via a certain mean field as

$$V_{res_l}(r,t)\Big|_{r\ge d_l(t)} \equiv 0 \qquad (2.7)$$

and, consequently,

$$f_l(r,t)\Big|_{r\ge d_l(t)} \equiv 1 \qquad (2.8)$$

with range parameters $d_l(t)$ to be determined below, but certainly small (In principle, we could choose them at will depending on what part of the bare interaction we want to consider explicitly).

Thus, we have to consider U to be the time-dependent potential which comes out in a solution of a corresponding TDHF problem

$$i\hbar\,\dot{\phi}_i = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + U\right]\phi_i \qquad (2.9)$$

with readjusted Skyrme force parameters.

We now proceed to the derivation of evolution equations for the single-particle orbitals ϕ_i and the correlation functions f_l in a self-consistent manner invoking a least action principle. In this approach one seeks solutions of

$$\delta\int_{t_1}^{t_2} dt\ \mathcal{L}\left[\Psi(t),\dot{\Psi}(t)\right] = 0 \qquad (2.10)$$

with the Lagrangian

$$\mathcal{L}\left[\Psi(t),\dot{\Psi}(t)\right] = \langle\Psi(t)\,|\,i\hbar\frac{\partial}{\partial t} - H\,|\,\Psi(t)\rangle \quad . \qquad (2.11)$$

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Before performing the variation simultaneously with respect to the functions f_ϱ and ϕ_i we have to simplify the very complicated expression (2.11).

A first step in this direction is the restriction to a consideration of correlations between nearest neighbours only, requiring that higher order effects, i.e., correlations between distant neighbours, which are known to have a weight of the order of 10% in the nuclear binding energy[5], contribute only to the mean field readjusted in the sense mentioned above. Thus, we do not neglect them at all but consider them in the same fashion as the mean-field theory does in all orders. For finite nuclear systems traditional cluster-expansion procedures can provide the framework for evaluating mean values of any operator $\langle O\rangle = \langle\Psi|O|\Psi\rangle$ with CBF's (see for example ref.[7] and references cited therein).

We apply the so-called Factor-Aviles-Hartog-Tolhoek (FAHT) expansion[11] in lowest order to eq. (2.11) arriving at (compare ref.[10])

$$\mathcal{L} \approx \mathcal{L}^{(2)}_{FAHT} \approx \sum_i \langle i|i\hbar\frac{\partial}{\partial t} - H_1(1,t)|i\rangle$$

$$-\Big\{\sum_{i<j}\langle ij|i\hbar\frac{\partial}{\partial t} - H_1(1,t) - H_1(2,t)|ij-ji\rangle \qquad (2.12)$$

$$-\sum_{i<j}\langle ij|F^+(12,t)\big[i\hbar\frac{\partial}{\partial t} - H_1(1,t) - H_1(2,t) - V_{res}(12,t)\big]F(12,t)|ij-ji\rangle\Big| \quad r_{12}\le d(t)$$

with $d(t) = \max_\varrho\{d_\varrho(t)\}$. The last two terms in eq. (2.12) would cancel if $d(t)\to 0$, i.e., we would arrive at the "TDHF Lagrangian". For nonvanishing values of the parameters $d(t)$ eq. (2.12) can be interpreted as a subtraction of the mean-field contribution of two particles at small distances combined with the addition of the corresponding correlated term. The energy functional obviously has the same structure.

Now, for simplicity, we assume a spin-isospin symmetric system and perform all the spin and isospin sums in eq. (2.12). In the following we denote the remaining spatial quantum numbers by μ, ν etc. The appearing spatial symmetric and antisymmetric uncorrelated two-particle wave functions $|\mu\nu\rangle$ and $|\mu\nu-\nu\mu\rangle$ as well as the combination $U(\vec r_1,t)+U(\vec r_2,t)$ appearing in eq. (2.15) we decompose into a Taylor expansion series around the center of mass position $\vec R = \frac{1}{2}(\vec r_1+\vec r_2)$ of the two particles of relative distance $\vec r = \vec r_1 - \vec r_2$. For a fixed $\vec R$ the integration over $\vec r$ in eq. (2.12) involves only single-particle orbitals ϕ_ν, ϕ_μ in a small volume of radius $\frac{1}{2}d(t)$

centered at $\vec R$. In this region the functions f_ϱ change rapidly from zero to unity but the mean field as well as the functions ϕ_ν should change rather smoothly. Therefore, it should be a valuable approximation to truncate the Taylor expansion series at some low order. In any practical case one should examine very carefully the question which order is reasonable. In the present paper, to demonstrate the structure of the equations of motion, we retain only the lowest order terms of the Taylor expansion. Higher order terms do not add qualitatively new aspects but may be important in the quantitative sense[10]. The main advantage of the truncation of the Taylor series at finite order is to have an explicit separation of the $\vec r$ and $\vec R$ dependence at small distances so that one is able to perform an integration over the angles $\hat r$ in eq. (2.12).

Performing all these operations we arrive at an approximate expression for the Lagrangian used in the following

$$\mathcal{L} \approx 4\Big\{\sum_{\nu=1}^{\frac{1}{2}A}\langle\nu|i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\vec\nabla^2 - U(\vec r,t)|\nu\rangle + i\hbar\sum_{\mu,\nu=1}^{\frac{1}{2}A}\xi^\circ_{\mu\nu}(t)\langle\mu|\nu\rangle$$

$$-\alpha_0(t)\Big[i\hbar\gamma_0(t) + \frac{\hbar^2}{4m}\delta_0(t) - 2\eta_0(t)\Big] + \frac{24\pi}{(A-1)}\eta_0(t)\int_0^{d_0(t)} r^2 f_0^2(r,t)\,dr \qquad (2.13)$$

$$+12\pi\beta_0(t)\int_0^{d_0(t)} r^2\Big[i\hbar f_0(r,t)\dot f_0(r,t) - \frac{\hbar^2}{m}\big(f_0'(r,t)\big)^2 - V_0(r)\,f_0(r,t)\Big]\Big\}$$

with

$$\alpha_0(t) = 12\pi\Big(\frac{d_0^3(t)}{3} - \int_0^{d_0(t)} r\,f_0^2(r,t)\,dr\Big) \qquad (2.14)$$

and

$$\begin{pmatrix}\beta_0(t)\\ \gamma_0(t)\\ \delta_0(t)\\ \eta_0(t)\end{pmatrix} = \frac{1}{2}\sum_{\mu,\nu=1}^{\frac{1}{2}A}\int d\vec R\;\phi^*_\mu(\vec R,t)\phi^*_\nu(\vec R,t)\begin{pmatrix}1\\ \frac{\partial}{\partial t}\\ \vec\nabla^2\\ U(\vec R,t)\end{pmatrix}\phi_\mu(\vec R,t)\,\phi_\nu(\vec R,t) \qquad (2.15)$$

Here the index „0" stands for the relative s-wave which is the only partial wave remaining in our lowest order considerations after the action of the projectors P_ϱ (see eq. (2.2)) in eq. (2.12). In eq. (2.21) we have introduced additional Lagrange multipliers $\xi^\circ_{\mu\nu}$ which

have to restore[10] the conservation of the single-particle wave function overlap matrix $\langle\mu|\nu\rangle$ in time

$$\frac{d}{dt}\langle\mu|\nu\rangle = 0 \quad , \tag{2.16}$$

or, if starting with orthonormal orbitals ϕ_ν at time $t=0$,

$$\langle\mu|\nu\rangle = \delta_{\mu\nu} \tag{2.17}$$

at any time t .

Starting from eqs. (2.13)-(2.15) a simultaneous variation with respect to the functions f_ℓ and ϕ_ν^* with

$$\dot{\beta}_0(t) = 2\,Re\,\gamma_0(t) \tag{2.18}$$

following directly from eq. (2.15), gives

$$\left[-\hbar\frac{Im\,\gamma_0(t)}{\beta_0(t)}\right] f_0(r,t) = -\frac{\hbar^2}{m}\left[\vec{\nabla}^2 + \frac{\delta_0(t)}{4\beta_0(t)}\right] f_0(r,t) + \left[V_0(r) + \frac{2(A-2)}{(A-1)}\,\frac{\eta_0(t)}{\beta_0(t)}\right] f_0(r,t) \tag{2.19}$$

and

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\vec{\nabla}^2 - U(\vec{r},t)\right]\phi_\nu(\vec{r},t) = \hat{I}_0\,\phi_\nu(\vec{r},t) - i\hbar\sum_{\mu=1}^{\frac{1}{2}A}\xi^0_{\nu\mu}(t)\,\phi_\mu(\vec{r},t) \tag{2.20}$$

with

$$\xi^0_{\nu\mu}(t) = \frac{1}{2}\frac{\partial}{\partial t}\left\{\alpha_0(t)\sum_{k=1}^{\frac{1}{2}A}\int d\vec{R}\,\left|\phi_k(\vec{R},t)\right|^2\phi^*_\mu(\vec{R},t)\,\phi_\nu(\vec{R},t)\right\} \quad , \tag{2.21}$$

$$\hat{I}_0 = \alpha_0(t)\sum_{\mu=1}^{\frac{1}{2}A}\phi^*_\mu(\vec{r},t)\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{4m}\vec{\nabla}^2 - 2U(\vec{r},t)\right]\phi_\mu(\vec{r},t) + 12\pi\sum_{\mu=1}^{\frac{1}{2}A}\left|\phi_\mu(\vec{r},t)\right|^2\int_0^{d_0(t)} R^2\left[V_0(R)f_0^2(R,t) + \frac{\hbar^2}{m}\left(f_0'(R,t)\right)^2 - i\hbar\,f_0\dot{f}_0\right]dR - \frac{24\pi}{(A-1)}\int_0^{d_0(t)} R^2 f_0^2(R,t)\,dR\sum_{\mu=1}^{\frac{1}{2}A}\phi^*_\mu(\vec{r},t)\,U(r,t)\,\phi_\mu(\vec{r},t) \tag{2.22}$$

Eqs. (2.19) formally resemble a Schrödinger equation with an "energy" given by the coefficient $-\hbar\,Im\,\gamma_0(t)/\beta_0(t)$, determined mainly by the single-particle orbitals (eqs. (2.15)), which in turn are coupled to the correlation function f_0 according to eqs. (2.20). The first term on r.h.s. is a correlational kinetic energy term while the second term represents a kinetic energy term connected with the uncorrelated motinn of a pair. In higher order a cross term would appear, the form of which, however, crucially depends on the truncation. The potential term consists of two parts: the bare potential in the s - channel and a time-dependent potential which is determined by the mean field (compare eq. (2.15)). For a system of only A=2 particles the second potential term vanishes, as it should, because its relative motion does not proceed in a medium of some other particles. Eqs. (2.19) are, however, not to be viewed as an eigenvalue problem but rather as second order differential equations in the coordinate r with two boundary conditions.

It can be shown that one of the two independent solutions of eqs. (2.19) is singular at $r = r_c$ ($r=0$ for a soft-core potential). The second, however, is well behaved and the function f_0 as well as its first derivatives are non-negative in this point[10]. Therefore, one can start the numerical integration at $r = r_c$ (or 0) with any small value of the quantity f_0 . According to the behaviour of the potential it will then increase rapidly with increasing r and reach a certain point $r = d_0(t)$ with $f_0'(r=d_0(t),t) > 0$. This point gives us the definition of the time-dependent range parameter $d_0(t)$, which possibly does not vary very strongly with time. After that we renormalize the function $f_0(r,t)$ to be equal to unity at this point. Such a procedure is equivalent to the boundary conditions

$$f_0(r = d_0(t), t) = 1 \tag{2.23}$$

$$f_0'(r = d_0(t), t) = 0 \tag{2.24}$$

which complete eqs. (2.19).

It should be mentioned in passing that by the outlined procedure the relation

$$0 \le f_0(r,t) \le 1 \tag{2.25}$$

is automatically fulfilled. It is equivalent to not allow the attractive part of the potential to have a large effect on the form of the

correlation function f_0, i.e., it supresses a corresponding "overshooting" before it asymptotically reaches unity. However, it has been shown that at least in the case of nuclear matter and for not too small densities the constraint (2.25) is either fulfilled or the deviations are small[12]. On the other hand by obeying the relation (2.25) we get rid of some time-dependent version of the so-called "Emery Difficulty"[12].

From eqs. (2.21), (2.22) it can be easily shown that the evolution equations for the single-particle orbitals (2.20) lead to TDHF (eqs. (2.9)) in the limit $d_0(t) \to 0$. The inclusion of higher partial waves yields additional terms of the type $\vec{I}_\ell$ and $\xi^\ell_{\nu\mu}$ in the r.h.s. of eqs. (2.20) with a structure similar to $\vec{I}_0$, $\xi^0_{\nu\mu}$.

Finally, it is useful to rewrite eqs. (2.19)-(2.22) in the form

$$i\hbar\Big[\dot{\phi}_\nu + \sum_{\mu=1}^{\frac{1}{4}A} \xi^0_{\nu\mu}(t)\,\phi_\mu - \alpha_0(t) \sum_{\mu=1}^{\frac{1}{4}A} \phi^*_\mu \frac{\partial}{\partial t}\phi_\mu \phi_\nu + 12\pi \int_0^{d_0(t)} R^2 f_0(R,t) \dot{f}_0(R,t)\,dR \sum_{\mu=1}^{\frac{1}{4}A} |\phi_\mu|^2 \phi_\nu\Big] = H_{eff}\,\phi_\nu \tag{2.26}$$

collecting all time-derivative terms in the l.h.s., with an obvious definition of the "effective" Hamiltonian H_{eff}. Then, the energy functional of the correlated system within our approximations can be written as

$$\mathcal{H} = \langle \Psi(t)|H|\Psi(t)\rangle = \sum_{\nu=1}^{\frac{1}{4}A} \langle \nu|H_{eff}|\nu\rangle = \mathcal{H}[\{\varphi_\nu\},\{\phi_\nu\},f_0] \tag{2.27}$$

which can also be extracted directly from eq. (2.13) omitting all time derivatives coming from $i\hbar\langle\Psi|\dot{\Psi}\rangle$ in eq. (2.11).

Returning to the philosophy outlined at the beginning of this section we summarize the scheme of the proposed method as follows:

i) Adjust the parameters of the effective two-body interaction to gross properties of the nuclear system under consideration using the energy functional (2.27) of the correlated system in the stationary case. This probably requires a several times simultaneous solution of a corresponding HF problem since its solution enters eq.(2.27) via the HF mean field defined by the HF orbitals φ_ν.

ii) Perform a TDHF calculation of the process using these readjusted parameters to get the time evolution of the mean field appearing in eqs. (2.19) and (2.20).

iii) Solve eqs. (2.19), (2.20) with the boundary conditions (2.23), (2.24).

To complete this section we emphasize that the total energy of the system (eq. (2.27)) can be shown to be conserved exactly by derivation (see ref.[10]).

3. Stationary Case and Initial Conditions

Starting with the solution of the stationary HF problem

$$\varphi_\nu(\vec{r},t) = \tilde{\varphi}_\nu(\vec{r})\exp\{-\tfrac{i}{\hbar}\varepsilon^{HF}_\nu t\} \tag{3.1}$$

it can be straightforwardly seen that an ansatz

$$\phi_\nu(\vec{r},t) = \tilde{\phi}_\nu(\vec{r})\exp\{-\tfrac{i}{\hbar}a_\nu t\} \tag{3.2}$$

makes the effective Hamiltonian H_{eff} stationary and the function $f_0(r,t)$ becomes a time-independent function $\tilde{f}_0(r)$ which in turn is defined now by

$$\frac{\tilde{\gamma}_0}{\tilde{\beta}_0}\tilde{f}_0(r) = -\frac{\hbar^2}{m}\Big[\vec{\nabla}^2 + \frac{\tilde{\delta}_0}{4\tilde{\beta}_0}\Big]\tilde{f}_0(r) + \Big[V_0(r) + \frac{2(A-2)}{(A-1)}\frac{\tilde{\eta}_0}{\tilde{\beta}_0}\Big]\tilde{f}_0(r), \tag{3.3}$$

where $\tilde{\beta}_0, \tilde{\delta}_0, \tilde{\eta}_0$ are given by replacing ϕ_ν by $\tilde{\phi}_\nu$ in eq. (2.15) and

$$\tilde{\gamma}_0 = \sum_{\mu,\nu=1}^{\frac{1}{4}A} a_\nu \int d\vec{R}\,|\tilde{\phi}_\mu(\vec{R})\tilde{\phi}_\nu(\vec{R})|^2. \tag{3.4}$$

The single-particle energies a_ν of the correlated system introduced in eq. (3.2) are connected with the eigenvalues ε_ν and the eigenfunctions $\tilde{\phi}_\nu$ of the stationary effective Hamiltonian $\tilde{H}_{eff}$

$$\tilde{H}_{eff}\,\tilde{\phi}_\nu(\vec{r}) = \varepsilon_\nu\,\tilde{\phi}_\nu(\vec{r}) \tag{3.5}$$

via

$$\varepsilon_\nu = a_\nu - \tilde{\alpha}_0 \sum_{\mu=1}^{\frac{1}{4}A} (a_\nu + a_\mu)\int d\vec{R}\,|\tilde{\phi}_\mu(\vec{R})\tilde{\phi}_\nu(\vec{R})|^2 \tag{3.6}$$

as can easily be deduced from eq. (2.26) with $\dot{\tilde{f}}_0 = 0$.

Thus, the stationary single-particle functions $\tilde{\phi}_\nu(\vec{r})$ as well as the stationary correlation function $\tilde{f}_0(r)$ are found by simultaneously solving eq. (3.3), diagonalizing the stationary effective Hamiltonian $\tilde{H}_{eff}$ and inverting the algebraic system of eqs. (3.6).

In order to propose appropriate initial conditions for solving the "correlated TDHF" equations derived in sect. 2, we check now, whether a Galilean translation of the stationary solutions $\tilde{\phi}_\nu(\vec{r})$, $\tilde{f}_0(r)$ is a solution of the time-dependent problem (2.19), (2.20). Introducing

$$\varphi_\nu^{tr}(\vec{r},t) = \tilde{\varphi}_\nu(\vec{r}-\vec{v}t)\exp\left\{-\frac{i}{\hbar}\left[(\varepsilon_\nu^{HF}+\tfrac{m}{2}v^2)t - m\vec{v}\vec{r}\right]\right\}, \tag{3.7}$$

$$\phi_\nu^{tr}(\vec{r},t) = \tilde{\phi}_\nu(\vec{r}-\vec{v}t)\exp\left\{-\frac{i}{\hbar}\left[(a_\nu+\tfrac{m}{2}v^2)t - m\vec{v}\vec{r}\right]\right\} \tag{3.8}$$

it is easy to show that

$$\begin{pmatrix}\beta_0^{tr}(t)\\ \eta_0^{tr}(t)\end{pmatrix} = \begin{pmatrix}\tilde{\beta}_0\\ \tilde{\eta}_0\end{pmatrix}, \tag{3.9}$$

$$\gamma_0^{tr}(t) = -\frac{i}{\hbar}\left[\tilde{\gamma}_0 + mv^2\tilde{\beta}_0\right] - \frac{1}{2}\vec{v}\sum_{\mu,\nu=1}^{\frac{1}{2}A}\int d\vec{R}\,\tilde{\phi}_\mu^*\tilde{\phi}_\nu^*\vec{\nabla}\tilde{\phi}_\mu\tilde{\phi}_\nu, \tag{3.10}$$

$$\delta_0^{tr}(t) = \tilde{\delta}_0 - \frac{4m^2v^2}{\hbar^2}\tilde{\beta}_0 + \frac{2im\vec{v}}{\hbar}\sum_{\mu,\nu=1}^{\frac{1}{2}A}\int d\vec{R}\,\tilde{\phi}_\mu\vec{\nabla}\tilde{\phi}_\nu^*\vec{\nabla}\tilde{\phi}_\mu\tilde{\phi}_\nu. \tag{3.11}$$

Introduction of eqs. (3.9)-(3.11) into eqs. (2.19) immediately yields

$$f_0^{tr}(r,t) = \tilde{f}_0(r) \tag{3.12}$$

which can be shown to hold also if higher partial waves are involved. A somewhat more tedious but simple procedure shows that by inserting eqs. (3.7), (3.8), (3.12) into the time-dependent equations (2.20) and making use of eqs. (3.6), one is led to the stationary equations (3.5). Thus, we have shown that initial conditions

$$\phi_\nu(\vec{r},t=0) = \tilde{\phi}_\nu(\vec{r})\exp\left\{\pm\frac{i}{\hbar}m\vec{v}\vec{r}\right\}, \tag{3.13}$$

$$f_0(r,t=0) = \tilde{f}_0(r) \tag{3.14}$$

similar to the ones conventially used in the TDHF initial value problem can be used to describe a heavy ion reaction.

4. The One-Particle Density Matrix

In order to evaluate the one-particle density matrix $\varrho(\vec{r},\vec{r}';t)$ we write it in the form

$$\varrho(\vec{r},\vec{r}';t) = \langle\Psi(t)|\sum_i \delta(\vec{r}_i-\vec{r})\hat{Q}_i(\vec{r}')|\Psi(t)\rangle \tag{4.1}$$

with $\hat{Q}_i(\vec{r}')$ defined by

$$\hat{Q}_i(\vec{r}')\Psi(\vec{r}_1,\dots,\vec{r}_i,\dots,\vec{r}_A) = \Psi(\vec{r}_1,\dots,\vec{r}',\dots,\vec{r}_A) \tag{4.2}$$

which is obviously equivalent to the usual definition. In lowest order of the FAHT cluster expansion, we get

$$\varrho(\vec{r},\vec{r}';t) = 4(2-A)\sum_{\nu=1}^{\frac{1}{2}A}\phi_\nu^*(\vec{r},t)\phi_\nu(\vec{r}',t) + \frac{2\binom{A}{2}\sum_{i<j}\langle ij|F^+(12,t)\delta(\vec{r}_1-\vec{r})\hat{Q}_1(\vec{r}')F(12,t)|ij-ji\rangle}{\sum_{i<j}\langle ij|F^+(12,t)F(12,t)|ij-ji\rangle} \tag{4.3}$$

Using the same approximations as in sect. 2, we get

$$\varrho(\vec{r},\vec{r}';t) = 4(2-A)\sum_{\nu=1}^{\frac{1}{2}A}\phi_\nu^*(\vec{r},t)\phi_\nu(\vec{r}',t) + 2\binom{A}{2}\frac{\left[2(A-1)\sum_{\nu=1}^{\frac{1}{2}A}\phi_\nu^*(\vec{r},t)\phi_\nu(\vec{r}',t) - \sum_{\mu,\nu=1}^{\frac{1}{2}A}B_{\mu\nu}^0(\vec{r},\vec{r}';t)\right]}{\left[\binom{A}{2} - 4\alpha_0(t)\beta_0(t)\right]} \tag{4.4}$$

with

$$B_{\mu\nu}^0(\vec{r},\vec{r}';t) = 6\left\{\int_{V_{10}(\vec{r},\vec{r}';t)} d\vec{r}_2\;\phi_\mu^*\left(\tfrac{\vec{r}+\vec{r}_2}{2},t\right)\phi_\nu^*\left(\tfrac{\vec{r}+\vec{r}_2}{2},t\right)\right.$$
$$\times\left[1-f_0(|\vec{r}'-\vec{r}_2|,t)f_0(|\vec{r}'-\vec{r}_2|,t)\right]\phi_\mu\left(\tfrac{\vec{r}'+\vec{r}_2}{2},t\right)\phi_\nu\left(\tfrac{\vec{r}'+\vec{r}_2}{2},t\right) \tag{4.5}$$
$$\left.+\left[\int_{V_{10}(\vec{r},\vec{r}';t)} d\vec{r}_2\,\phi_\mu^*\left(\tfrac{\vec{r}+\vec{r}_2}{2},t\right)\phi_\nu^*\left(\tfrac{\vec{r}+\vec{r}_2}{2},t\right)\left[1-f_0(|\vec{r}'-\vec{r}_2|,t)\right]\phi_\mu(\vec{r}_2,t)\phi_\nu(\vec{r}',t) + h.c.\right]\right\}.$$

Here the integration limits are

$$V_{10}(\vec{r},\vec{r}';t) \;\hat{=}\; |\vec{r}-\vec{r}_2| \le d_0(t)\,,\ |\vec{r}'-\vec{r}_2| > d_0(t)\quad;$$
$$V_{20}(\vec{r},\vec{r}';t) \;\hat{=}\; |\vec{r}-\vec{r}_2| \le d_0(t)\,,\ |\vec{r}'-\vec{r}_2| \le d_0(t)\,. \tag{4.6}$$

The expressions (4.4), (4.5) show that the one-particle density matrix is indeed hermitean

$$\rho(\vec{r},\vec{r}',t) = \rho^*(\vec{r}',\vec{r},t) \quad . \tag{4.7}$$

Furthermore, considering the diagonal part $\rho(\vec{r},\vec{r},t)$ only, the integral over V_{10} in eq. (4.5) vanishes and the integral over V_{20} ranges over a sphere of radius $d_0(t)$ centered at $\vec{r}$. Therefore, if integrating eq. (4.4) over $\vec{r}$, the numerator and denominator cancel so that

$$\int \rho(\vec{r},t)\, d\vec{r} = A \tag{4.8}$$

at any time. This property in turn is a general advantage of the FAHT cluster expansion and holds order by order[11].

In order to further simplify expression (4.4) one could decompose once more the quantities ϕ_ν in the small integration volumes (4.6), i.e., in lowest order, replace $\vec{r}_2$ by $\vec{r}$ in the arguments of ϕ_ν in the region V_{10} and by $\frac{1}{2}(\vec{r}+\vec{r}')$ in the region V_{10} . In this case the integrations over the angles $\hat{r}_2$ can be even performed analytically in the region V_{10} (but not yet in V_{20}). In this additional crude approximation the diagonal part of the density matrix takes the simple form

$$\rho(\vec{r},t) \approx 4(2-A) \sum_{\nu=1}^{\frac{1}{2}A} |\phi_\nu(\vec{r},t)|^2 + 4\binom{A}{2} \frac{[(A-1)\sum_{\nu=1}^{\frac{1}{2}A} |\phi_\nu(\vec{r},t)|^2 - \sum_{\mu,\nu=1}^{\frac{1}{2}A} |\phi_\mu(\vec{r},t)|^2 |\phi_\nu(\vec{r},t)|^2 \alpha_0(t)]}{[\binom{A}{2} - 4\alpha_0(t)\beta_0(t)]} \tag{4.9}$$

obviously also obeying eq. (4.8). In the limit $d_0(t) \to 0$ (that is, $f_0 \to 1, \forall r$) we get from eq. (4.4)

$$\rho(\vec{r},\vec{r}',t) = 4 \sum_{\nu=1}^{\frac{1}{2}A} \phi_\nu^*(\vec{r},t)\phi_\nu(\vec{r}',t) , \tag{4.10}$$

i.e., the TDHF density matrix.

We emphasize that if one calculates from eq. (4.4) the density matrix $\rho_{\mu\nu}(t)$ using either the functions ϕ_ν or the TDHF orbitals f_ν as a time-dependent basis completed by evolving also the corresponding functions for unoccupied states, one gets

$$\dot{\rho}_{\mu\nu}(t) \neq 0 \tag{4.11}$$

and, in particular, the occupation numbers $\rho_\mu(t)$ are no more constant in time as in usual TDHF. This does not contradict the statement that equations (2.18), (2.20) are invariant under time reversal. That is, by solving these equations with initial conditions of the type (3.13), (3.14) up to a certain time t and then going back, one would arrive at the initial state of the system at $t=0$. This situation is similar to the TDHF case: In the stationary HF basis it is known that eq. (4.11) holds too, although TDHF is time reversal invariant on the microscopic level. In our case eq. (4.11) involves particle-hole excitations even in the TDHF basis caused by the inclusion of short-range correlations.

Finally it should be pointed out, that with eq. (4.4) one has the possibility to calculate the evolution of the momentum distribution (the Wigner transform of the density matrix) which is expected to have large momentum components and should be examined in the future with respect to a possible dynamical realization of SRC's as discussed in the introduction.

5. Summary

We have demonstrated an extension of the TDHF method to deal in lowest order with two-body correlations of short range assuming higher order effects as well as effects of LRC's being sufficiently described by a mean field which comes out from a solution of the corresponding TDHF problem with readjusted parameters of the effective interaction. The method was demonstrated for the lowest order contributions to the relative s - wave only.

In principle, three-body clusters could be involved analogously, by investigating the next order of the FAHT cluster expansion. This, however, would lead to a much more complicated theory possibly not suitable for numerical investigations at all.

The use of a more realistic potential including spin-orbit and tensor forces is possible. As a consequence we would have to consider a larger number of correlation functions f_{jst} and end up with a system of directly coupled equations for them instead of eq. (2.19) for each separate ℓ .

Further simplifications of the proposed formalism are desirable. One of them could be the derivation of some kind of viscous hydrodynamics by methods similar to those used to derive non-viscous hydrodynamics from TDHF (compare, e.g., ref.[2]). Another possibility of an essential reduction of the derived equations is to restrict the model functions ϕ_ν from the outset to be the TDHF orbitals and to solve "only" an ordinary TDHF problem together with

eqs. (2.19) which are not so difficult to handle. One could also try to guess the form of the correlation functions f_e or take them time-independent in a simple form as in many phenomenological applications of the Jastrow approach in the stationary problem (for an example see ref.[5]). It should, however, be pointed out, that along this line problems with the energy conservation arise, since the basic ingredients of the theory are no more taken from a self-consistent variational problem.

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Мэдлер П.
E4-82-693

Короткодействующие корреляции в обобщенной теории среднего поля с зависимостью от времени

Осуществляется обобщение зависящей от времени теории среднего поля на уровне микроскопической обратимости путем включения сильных короткодействующих корреляций, исходя из реалистических нуклон-нуклонных сил. На основе принципа наименьшего действия для скоррелированных пробных волновых функций выводятся уравнения движения для корреляционных функций и одночастичных модельных волновых функций в низшем порядке кластерного разложения типа FAHT. Эффекты более высокого порядка и корреляции дальнего действия рассматриваются только в той мере, в которой они дают вклад в среднее поле через переопределенное эффективное двухчастичное взаимодействие. Исследуется соответствующая стационарная задача и предлагаются подходящие начальные условия для описания тяжелоионной реакции. Выводится выражение для одночастичной матрицы плотности.

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Mädler P.
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Short-Range Correlations in an Extended Time-Dependent Mean-Field Theory

An extension is performed of the time-dependent mean-field theory by an explicit inclusion of strong two-body correlations of short range on a level of microscopic reversibility relating them to realistic nucleon-nucleon forces. Invoking a least action principle for correlated trial wave functions, equations of motion for the correlation functions and the single-particle model wave function are derived in lowest order of the FAHT cluster expansion. Higher order effects as well as long-range correlations are consider only to the extent to which they contribute to the mean field via a readjusted phenomenological effective two-body interaction. The corresponding correlated stationary problem is investigated and appropriate initial conditions to describe a heavy ion reaction are proposed. The singleparticle density matrix is evaluated.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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