QUANTUM STATISTICAL APPROACH TO EXTENDED MEAN-FIELD THEORY

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The time-dependent Hartree-Fock theory is generalized in order to include two-body collisions. Using the projection operator techniques of statistical mechanics a transport equation is derived for the uncorrelated part of the full A-particle density matrix. This leads to an equation of motion for the one-particle density matrix which includes a collision term. The collision term is considered in the weak-coupling limit and a master equation is obtained for the occupation probabilities of the single-particle levels.

1. INTRODUCTION

Inclusion of two-body collisions in a self-consistent mean-field description is a natural step in developing a unique understanding of low-energy nuclear dynamics. For this purpose, recently, several attempts have been made to derive the extended time-dependent Hartree-Fock equations /1-6/. In the present work this problem is studied in the frame of statistical mechanics. Using the well known Projection Operator Techniques we derive a transport equation for the single-particle density matrix.

The use of projection operator techniques to derive transport equations has become increasingly more common in recent years /7,8/. Although these techniques are very general they have been especially useful in problems where systems are in contact with reservoirs or where one is interested only in the diagonal matrix elements of the density matrix in some representation. In these problems the degrees of freedom of the reservoirs or the off-diagonal part of the density matrix are considered to be irrelevant and the irrelevant part of the density operator is formally eliminated. One is then left with an exact equation for the remaining relevant part of the density operator. However, in many problems involving coupled dynamical systems it is necessary to have a description where each degree of freedom is considered to be on an equal footing. In this work we derive a transport equation for the coupled A-particle system where the irrelevant degrees of freedom are not the dynamical degrees of freedom of the system but rather the correlations between particles produced by the interactions. The correlations are formally eliminated and we obtain an exact equation for the relevant part of the A-particle density operator. This yields, for the one-particle density matrix, an equation motion which includes a collision term /4/.

2. EXTENDED MEAN-FIELD EQUATIONS

We consider an interacting A-particle system with the total Hamiltonian

$$H = \sum_{i}^{A} \frac{1}{2m} p_i^2 + \sum_{i<j}^{A} v(i,j) \tag{2.1}$$

where the first and second terms denote the kinetic energy and the two-body interactions of the particles. The time evolution of the system is determined by the Liouville equation,

$$i \frac{\partial}{\partial t} F(t) = [H, F(t)] \equiv LF(t) \tag{2.2}$$

where $F(t) = F(12\cdots A, 1'2'\cdots A';t)$ is the exact A-particle density matrix and $1\cdots A$ abbreviates the coordinates including spin-isospin of the particles. The one-particle density matrix $\rho(t)$ is obtained from A-particle density matrix by taking trace over the subspace corresponding to A-1 particles,

$$\begin{aligned} \rho(11';t) &= \mathrm{Tr}\,\{F(t)\}_{A-1} \\ &= \int\cdots\int d2\cdots dA\, F(12\cdots A, 1'2\cdots A;t). \end{aligned} \tag{2.3}$$

In general the total density matrix can be written as the sum of two terms,

$$F(t) = F_0(t) + F_{cor}(t) \tag{2.4}$$

where $F_0(t)$ is the uncorrelated component and it is defined in terms of one-particle density matrices as

$$F_0(t) = \mathcal{A}\, \rho(11';t) \cdots \rho(AA';t) \tag{2.5}$$

with $\mathcal{A}$ is the antisymmetrization operator.

The second term in the r.h.s. of (2.4) as the correlated component of the total density matrix and it is given by the difference between the exact density matrix and the uncorrelated component.

The TDHF approximation to the many-body dynamics is obtained if the correlated component in (2.4) is neglected completely / 9/. This means that one assumes the factorization structure (2.5) for the total density matrix at all times. As a result, inserting (2.5) into (2.2) and taking trace over (A-1)-particle space we obtain TDHF equations

$$i \frac{\partial}{\partial t} \rho_{HF}(t) = [\mathcal{H}_{HF}(t), \rho_{HF}(t)], \tag{2.6}$$

for the one-particle density matrix. The self-consistent Hartree-Fock Hamiltonian is determined by

$$\mathcal{H}_{HF}(t) = \frac{p^2}{2m} + \mathrm{Tr}\, v\, \rho_{HF}(t). \qquad (2.7)$$

In general the many-body density matrix deviates from the factorized form (2.5) as a result of the correlations. In the following, using the projection operator techniques of statistical mechanics, we derive a generalized equation for the one-particle density matrix, in which the correlations are taken into account.

In the usual applications of the projection operator techniques in deriving transport equations, the degrees of freedom which corresponds to a part of the system or the off-diagonal part of the density matrix in some representation are regarded irrelevant. Then one obtains for the remaining relevant degrees of freedom an exact equation of motion by eliminating the irrelevant degrees of freedom with the use of properly defined projection operators /7,8/. In the problem of an interacting A-identical particles that we consider, all the dynamical degrees of freedom should be treated on an equal footing and consequently they cannot be seperated into relevant and irrelevant parts. However, the structure of (2.4) suggests that we can regard the uncorrelated component $F_0(t)$ as the relevant part and the correlated component $F_{cor}(t)$ as the irrelevant part of the total density matrix. Then in order to eliminate correlations we should define an operator $C(t)$ which projects the total density matrix on to the uncorrelated part. It can be seen that the integral operator which is defined as

$$C(t) = \mathcal{A} \sum_{J=1}^{A} \prod_{K\neq J}^{A} \rho(KK';t) \int dK-(A-1)\, \mathcal{A} \prod_{K=1}^{A} \rho(KK';t) \int dK \qquad (2.8)$$

has the right property and the application of $C(t)$ on the total density matrix

$$C(t)\, F(t) = F_0(t), \qquad (2.9)$$

gives the relevant part of the density matrix. Therefore $C(t)$ when it is applied to $F(t)$ behaves like a time dependent projection operator on the uncorrelated component. Similarly $Q(t)=1-C(t)$ acts like a projection operator on to the uncorrelated component. In addition $C(t)$ and $Q(t)$ have the property that although they are time dependent, they effectively commute with the time derivative,

$$C(t)\, \frac{\partial}{\partial t} F(t) = \frac{\partial}{\partial t} \left[C(t)F(t)\right] = \frac{\partial}{\partial t}\, F_0(t), \qquad (2.10)$$

and similarly for $Q(t)$.

Applying $C(t)$ and $Q(t)$ to both sides of (2.2) and using the property (2.10) we obtain two coupled equations for the correlated (irrelevant) and the uncorrelated (relevant) parts of the density matrix,

$$i \frac{\partial}{\partial t} F_o(t) = C(t)L \{F_o(t) + F_{cor}(t)\} \tag{2.11}$$

$$i \frac{\partial}{\partial t} F_{cor}(t) = Q(t)L \{F_o(t) + F_{cor}(t)\} \quad . \tag{2.12}$$

The second equation can be solved formally as

$$F_{cor}(t) = G(t,t_o)F_{cor}(t_o) - i \int_{t_o}^{t} dt' G(t,t')L_1(t')F_o(t') \tag{2.13}$$

where $L_1(t)$ denotes the Liouville operator corresponding to the residual interactions $V(t) = v - U(\rho)$, and $U(\rho)$ is the meanfield potential. The propagator $G(t,t')$ is given by

$$G(t,t') = T \cdot \exp\{-i \int_{t'}^{t} du\, Q(u)\, L\} \tag{2.14}$$

where T denotes the time-ordered integration due to the time dependence of Q. As seen from (2.13) the correlated part of density matrix consists of two contributions. The first term on the r.h.s. describes the propagation of initial correlations whereas the second term determines dynamical correlations produced by the residual interactions. Even initially there are no correlations, in this case the first term vanishes, the correlated part of the density matrix does not vanish as a result of the dynamical correlations. Eliminating the correlated component from the equation (2.11) we obtain a transport equation

$$i \frac{\partial}{\partial t} F_o(t) = CLF_o(t) - i \int_{t_o}^{t} dt' CL_1 G(t,t')L_1 F_o(t') \tag{2.15}$$

for the relevant part of the density matrix, where a term due to the initial correlations is omitted. We can immediately derive an equation for the one-particle density matrix by taking trace over the sub-space of (A-1) particles on both sides of (2.15). As a result we obtain a generalized equation for the one-particle density matrix as

$$i \frac{\partial}{\partial t} \rho(t) = [\mathcal{H}(t), \rho(t)] - iK(\rho) \tag{2.16}$$

which describes the single-particle motion under the influence of the mean field $\mathcal{H}(t)$ and the collision term $K(\rho)$. The collision term is given by

$$K(\rho) = \int_{t_o}^{t} dt'\, Tr\{L_1 G(t,t')L_1 F_o(t')\}_{A-1} \tag{2.17}$$

where Tr denotes integrations over the coordinates of (A-1)-particles. The equations (2.15) and (2.17) are in principle exact and they are obtained from the Liouville equation (2.2) by formal manipulations. However, they provide a general basis for including correlations and for going beyond the self-consisent meanfield description of the many-body dynamics. The collision term can be studied in different approximations. In low energy, the dynamic is mainly determined by the mean-field and the collision term can be considered in a weak coupling approximation. In high energy limit the collision term plays a dominant role. In fact for classical systems it can be shown that (2.17) reproduces the collisoin term of the Boltzmann equation /10/.

Before we go into the approximate evaluation of the collision term in the weak-coupling limit, we consider the expectation values of operators, in particular two-body operators, in the present formulation. The expectation value of an operator $\mathcal{O}$ by definition is given by

$$\langle \mathcal{O} \rangle (t) = \mathrm{Tr}\, \mathcal{O}\, F(t) \tag{2.18}$$

Using the decomposition (2.4), the expectation value can be expressed in terms of sums of two terms,

$$\langle \mathcal{O} \rangle (t) = \langle \mathcal{O} \rangle_0(t) - i \int_{t_0}^{t} dt' \langle \mathcal{O}\, G(t,t') L_1 \rangle_0(t') \tag{2.19}$$

where the result (2.13) is used for $F_{cor}(t)$ and $\langle \cdots \rangle_0 = \mathrm{Tr}(\cdots)F_0$ denotes the expectation value over the relevant part of the density matrix. As seen from (2.19) the expectation value of an operator can be given as the sum of the mean field contribution, which is the first term on the r.h.s. of (2.19), and the contribution arising from the correlations.

For one-body operators the contributions due to the correlations vanishes due to the fact that L_1 in (2.19) is a traceless two-body operator and a self-contraction does not contribute. But for a two-body operator, the contributions due to the correlations do not vanish in general. For example if the two-body interactions are taken as the operator $\mathcal{O} \to v$, the second term in (2.19) gives the correlation energy. In many cases, it may be more convenient to convert (2.19) into a differential equation. Taking time derivative and using (2.11) and (2.12) we obtain a differential equation

$$\frac{d}{dt} \langle \mathcal{O} \rangle = \langle -i \mathcal{O} \mathcal{L} \rangle_0 - \int_{t_0}^{t} dt' \langle \mathcal{O}\, L_1 G(t,t') L_1 \rangle_0 \tag{2.20}$$

for the rate of expectation value, where $\mathcal{L}$ denotes the Liouville operator corresponding to the mean-field Hamiltonian. This equation can be regarded as a

Langevin equation for the collective operator $\mathcal{P}$, in which the first term on the r.h.s. describes the driving force on $\mathcal{P}$ due to the mean field and the second term determines the dissipation. In fact, under certain approximations (2.20) can be converted into a classical equation of motion for the collective variables /11/.

3. WEAK-COUPLING LIMIT AND MASTER EQUATION

The collision term (2.17) provides a basis for introducing different approximations Here we consider the weak-coupling limit and evaluate the collision term by assuming some general statistical properties for the residual interactions (random two-body collisions). The collision term in general involves the two different characteristic times, (i) the decay time τ_λ, of the intermediate propagator G, which measures the average time interval between subsequent two-body collisions, (ii) the correlation time, τ_{cor}, of the residual interactions which corresponds to the duration time of a two-body collision. In low energy nuclear reactions, due to large mean free path, λ, of nucleons the time spent between subsequent collisions is much larger than the duration time of a collision. Consequently the weak coupling limit is defined by $\tau_{cor} \ll \tau_\lambda$ /12/. Classically this condition corresponds to a dilute gas limit and it can be expressed in terms of the range, σ, of the interactions and the mean free path as $\sigma \ll \lambda$. In the weak coupling limit the leading order contribution to the collision term is obtained by replacing the full propagator in (2.7) with the mean-field propagator,

$$K(\rho) = \int_{t_o}^{t} dt' \, Tr[V, g_o[V, F_o^{(4)}(t') g_o^+]], \tag{3.1}$$

where the mean-field propagator is given by

$$g_o(t,t') = T\cdot\exp\{-i \int_{t'}^{t} du \mathcal{H}(u)\} \tag{3.2}$$

and the uncorrelated part of A-particle density matrix $F_o = F_o^{(A)}$ is replaced by the uncorrelated part of 4-particle density matrix $F_o^{(4)}$, as a result of two-body character of the residual interactions. The approximate expression (3.1) for the collision term is still time reversible and it carries memory effects. However, inconsistent with the weak-coupling limit, it can be further simplified. We consider the correlation function,

$$\chi(t,t') = \langle V \, g_o(t,t') V \, g_o^+(t,t') \rangle_o \tag{3.3}$$

of the residual interactions. As a result of the random properties of the residual interactions, the correlation function decays over a time interval

$t-t' \sim \tau_{cor}$, which is defined as the correlation time /12/. The collision term has essentially the same structure as the correlation function and consequently the decay time of the collision kernel (memory time) is determined by the correlation time. The characteristic variations in the one-particle density matrix $\rho(t)$ take place over time intervals of order τ_λ. However, the variations of $\rho(t)$ during time intervals of order τ_{cor} and hence the memory effects in the collision term can be neglected in the weak-coupling limit. As a result, within the Markov approximation the collision term becomes as

$$K(\rho) = \int_0^\infty d\tau \quad Tr[V, [g_0 V g_0^+, F_0^{(4)}(t)]] \tag{3.4}$$

where the upper limit of the τ-integration is extended to infinity. Furthermore, if the variations of the mean field during time intervals of order τ_{cor} is neglected, the meanfield propagator is approximately given by

$$g_0(t,t-\tau) \cong \exp\{-i\tau \mathcal{H}(t)\}. \tag{3.5}$$

Introducing some random properties for the residual interaction and neglecting the memory effects in the collision term the equation (2.16) with $K(\rho)$ given by (3.4) becomes time irreversible and it describes the evolution of the system towards statistical equilibrium. In the derivation of collision term (3.4) the decay of the intermediate propagator G in (2.17) is neglected. However, it is possible to take the decay of the propagator into account and one obtains a mean-field propagator in(3.4) which is modified by a decay matrix /4/.

In the remaining part of this sectiion we use the extended mean-field equation (2.16) with the collision term (3.4) to derive a quantum mechanical master equation for the occupation probabilities of the single-particle states. We expand the one-body density matrix in terms of the complete set of TDHF single-particle states,

$$\rho(t) = \sum_{\alpha\beta} |\alpha(t)\rangle \rho_{\alpha\beta}(t) \langle\beta(t)| \tag{3.6}$$

where the single-particle states are determined by

$$i \frac{\partial}{\partial t} |\alpha(t)\rangle = \mathcal{H}(t) |\alpha(t)\rangle \tag{3.7}$$

The collision term in general is not diagonal in the TDHF representation. Hence the off-diagonal elements $\rho_{\alpha\beta}, \alpha \neq \beta$ of the density matrix do not vanish and they describe the non-statistical aspects of two-body collisions. We assume that the mean-field describes the essential coherent aspect of the single-particle motion and neglect the additional coherence introduced by the residual interactions.

Therefore in the following we neglect the off-diagonal elements. Inserting the expansion (3.6) into (2.16) we obtain a master equation for the occupation probabilities $\rho_{\alpha\alpha}(t)\equiv\rho_\alpha(t)$ of single-particle states,

$$\frac{\partial}{\partial t}\rho_\alpha = \sum W_{\alpha\beta,\gamma\delta}(t)\left[\rho_\gamma\rho_\delta(1-\rho_\alpha)(1-\rho_\beta)-\rho_\alpha\rho_\beta(1-\rho_\gamma)(1-\rho_\delta)\right] \tag{3.8}$$

where the transition probabilities are given by

$$W_{\alpha\beta,\gamma\delta}(t) = |V_{\alpha\beta,\gamma\delta}(t)|^2\pi\ \delta\left[\varepsilon_\alpha(t)+\varepsilon_\beta(t)-\varepsilon_\gamma(t)-\varepsilon_\delta(t)\right] \tag{3.9}$$

and $\varepsilon_\alpha(t)=\langle\alpha(t)|\mathcal{H}(t)|\alpha(t)\rangle$ denotes the diagonal elements of the mean-field Hamiltonian. If we include the decay of the intermediate propagator G in (2.17) into the calculation, as a result of finite width of single-particle states, we get a soft δ-function instead of δ-function in the transition probabilities.

4. CONCLUSIONS

We have formulated a theory in order to generalize the TDHF description by including consistently two-body collisions. In usual applications of the projection operator techniques of statistical mechanics, one derives transport equations for the relevant degrees of freedom by formally eliminating the degrees of freedom which are regarded irrelevant. Here we use these techniques to derive an exact equation for the uncorrelated component of the A-particle density matrix by eliminating the correlations from the equation of motion. By reducing the resulting equation to the single-particle degree of freedom, we obtain for the one-particle density matrix a generalized equation which includes a collision term. The exact collision term provides a basis for introducing approximations and for studying the equilibration processes in quantum and classical systems. For example for dilute classical systems one obtains the Boltzmann collision term. In the present work we consider the collision term in the weak-coupling limit and derive a quantal master equation for the single-particle occupation probabilities.

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