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Extended Time-Dependent Hartree-Fock Approximation with Particle Collisions

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We formulate an extended time-dependent Hartree-Fock approximation which includes particle collisions. As the configuration-space analog of the quantum Boltzmann equation, it can be utilized to study the dynamics of nuclear or other fermion systems when irreversible dissipation is present.

Recent renewed interest in the time-dependent Hartree-Fock approximation (TDHF) for the microscopic description of the dynamics of nuclear systems was pioneered by Bonche, Koonin, and Negele.[1] Since then, many TDHF calculations were carried out[2] and many different theoretical investigations were initiated.[2,3] However, in the TDHF approximation, the fermions are assumed to interact only through the mean field and the collisions between particles due to residual interactions are neglected. Because particle collisions are capable of altering the occupation probabilities and dissipating energies, the pattern of behavior of the quantum fluid can be that of hydrodynamics[4] or elastic response,[5,4] depending on the degree of particle collisions. A careful analysis of particle collision also helps our understanding of dissipative phenomena for which much progress has been made recently.[6] However, the incorporation of particle collisions into the TDHF approximation has, up to now, not been formulated.

Previous extension of the TDHF approximation was discussed in terms of a multideterminant representation and Pauli's master equation.[4] In this Letter, we present a different extended time-dependent Hartree-Fock approximation (ETDHF) in which collisions between particles are explicitly taken into account. The final set of equations turns out to be simple and physically transparent and may be of practical interest to those working in the field of the dynamics of nuclear or other fermion systems. Furthermore, concepts such as entropy, temperature, thermal equilibrium, and local equilibrium can be naturally and quantitatively introduced. The approach from nonequilibrium to thermal equilibrium can be quantitatively studied.

Being the configuration-space analog of the quantum Boltzmann equation, our set of equations should retain certain characteristics of the Boltzmann equation. It should be closed Markovian in the sense that all the quantities are to be specified at the same time coordinate.[7] This requirement necessitates an integration over the collision history analytically. Just as in the Boltzmann equation, we wish to keep terms only up to the second order in the residual interaction. Finally, as the Boltzmann equation violates time-reversal invariance, the latter concept needs to be properly introduced.

The starting point of our formulation is the

equation of motion for the Green's function[8,9] $g^<(1,1')$

$$\left[i\hbar \frac{\partial}{\partial t_1} + i\hbar \frac{\partial}{\partial t_{1'}} + \frac{\hbar^2}{2m} (\nabla_{r_1}{}^2 - \nabla_{r_{1'}}{}^2) - U_{\mathrm{MHF}}(1) + U_{\mathrm{MHF}}(1') \right] g^<(1,1') = I(1,1'), \tag{1}$$

where the argument 1 (and similarly 1') represents the collection of the spatial coordinate $\vec{r}_1$, the spin and isospin coordinate ξ_1, and the time coordinate t_1. The Green's function is defined as

$$ig^<(1,1') = -\langle \hat{\psi}^\dagger(1')\hat{\psi}(1)\rangle , \tag{2}$$

and

$$ig^>(1,1') = \langle \hat{\psi}(1)\hat{\psi}^\dagger(1')\rangle , \tag{3}$$

where the expectation value is taken with respect to the dynamical wave-packet–like state in question. The modified Hartree-Fock potential $U_{\mathrm{MHF}}(1)$ is given by

$$U_{\mathrm{MHF}}(1)g^<(1,1') = -i\int dx_2 v(x_1,x_2)\mathfrak{A}[g^<(1,1')g^<(2,2^+)]_{t_1=t_2}, \tag{4}$$

where

$$\mathfrak{A}[g^<(1,1')g^<(2,2^+)] \equiv g^<(1,1')g^<(2,2^+) - g^<(1,2^+)g^<(2,1'),$$

x represents $\vec{r}$ and ξ, and the symbol 2^+ implies $t_2{}^+ \geq t_2$. We envisage that the mean-field theory of TDHF, as obtained by using an effective interaction $v(x_1,x_2)$ and neglecting the collision matrix $I(1,1')$ in Eq. (1), is a good and approximate representation of the dynamics. It is now necessary to include the collision term involving only residual interaction $v'(x_1,x_2)$ between the fermions in the Born scattering approximation.

We shall specialize to a representation of the Green's function in the form

$$-ig^>(x_1,t_1;x_1',t_1') = \sum_\lambda^\infty n_\lambda(T)\psi_\lambda(x_1,t_1)\psi_\lambda{}^*(x_1',t_1'), \tag{5}$$

with the complementary Green's function

$$ig^>(x_1,t_1;x_1',t_1') = \sum_\lambda^\infty [1-n_\lambda(T)]\psi_\lambda(x_1,t_1)\psi_\lambda{}^*(x_1',t_1'), \tag{6}$$

where $T = \frac{1}{2}(t_1+t_1')$. The effect of particle collisions is readily separated by choosing the complete set of single-particle states ψ_λ's to satisfy the modified TDHF equation:

$$i\hbar \frac{\partial}{\partial t}\psi_\lambda(x,t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_{\mathrm{MHF}}(x,t)\right)\psi_\lambda(x,t), \tag{7}$$

where the potential U_{MHF} as defined by (4) is the same as the ordinary Hartree-Fock potential except that the occupation number is now time dependent. Such a choice of a complete set leads to

$$\frac{\partial}{\partial t} n_\lambda(t) = -(1/\hbar)\int dx_1 dx_1' \psi_\lambda{}^*(x_1,t) I(x_1,t;x_1',t^+)\psi_\lambda(x_1',t). \tag{8}$$

We complete our formulation by evaluating the right-hand side of the above equation. The evaluation proceeds as follows.

The equal-time collision matrix is given by[8,9]

$$I(x_1,t_1;x_1',t_1^+) = -i\int dx_2 [v'(x_1,x_2) - v'(x_1',x_2)]g_{2c}(1,2;1',2^+)|_{t_1'=t_1^+}, \tag{9}$$

where $t_1 = t_2$ and g_{2c} is the two-body Green's function due to particle collisions. As the hierarchy of equations coupling the different Green's functions are the same whether the Green's function is defined with respect to the dynamical wave-packet–like state or in terms of a grand canonical ensemble, the resultant perturbation expansion[10] of $g_{2c}(1,2;1',2^+)$ is the same as obtained previously by Martin and

Schwinger[8] and Kadanoff and Baym[9] which, up to the Born collision term, is given by

$$g_{2c}(1,2;1',2^+)=(i/\hbar)\int d\bar{x}_1 d\bar{x}_2 v'(\bar{x}_1,\bar{x}_2)\int_{-\infty}^{t_1^-} d\bar{t}_1\{\mathcal{A}[g^>(1,\bar{1})g^>(2,\bar{2})]g^<(\bar{1},1')g^<(\bar{2},2^+) - \mathcal{A}[g^<(1,\bar{1})g^<(2,\bar{2})]g^>(\bar{1},1')g^>(\bar{2},2^+)\}_{\bar{t}_2=\bar{t}_1}. \quad (10)$$

As in Kadanoff and Baym,[9] the resultant collision matrix will lead to a time-reversal violating Eq. (1). To integrate over $\bar{t}_1$, we shall consider the case in which the mean field is a slowly varying function of time. Furthermore, as the Green's function is expected to peak sharply about the relative time coordinate so that only a small region of $\bar{t}_1$ is important in the integral of (10), it is reasonable to assume there that the time dependence of the single-particle wave function satisfies the approximation

$$\psi_\lambda(x,T+\tfrac{1}{2}\tau)\cong\exp[-i\epsilon_\lambda(T)\tau/2\hbar]\psi_\lambda(x,T), \quad (11)$$

where $\epsilon_\lambda(T)=(\psi_\lambda(x,T), h(T)\psi_\lambda(x,T))$ and $h(T)$ is the modified Hartree-Fock single-particle Hamiltonian defined by Eq. (7). Such an approximation is found to account quite well the predominant time dependence of the TDHF single-particle wave functions for small time intervals of τ.[11] In a related manner, it is also reasonable to assume there that

$$\epsilon_\lambda(\tfrac{1}{2}(t_1+\bar{t}_1))\cong\epsilon_\lambda(t_1), \quad (12)$$

$$n_\lambda(\tfrac{1}{2}(t_1+\bar{t}_1))\cong n_\lambda(t_1). \quad (13)$$

From Eqs. (9) and (10, the result of the integration over $\bar{t}_1$ gives the equal-time collision matrix

$$I(x,t;x',t^+)=-i\int dx''[v'(x,x'')-v'(x',x'')]\sum_{1234}[(1-n_1)(1-n_2)n_3n_4-n_1n_2(1-n_3)(1-n_4)] \times[(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4-i\eta)^{-1}]_{\eta\to0}\psi_1(x,t)\psi_2(x'',t)\psi_3^*(x'',t)\psi_4^*(x',t)\langle1,2|v'|4,3-3,4\rangle|^2. \quad (14)$$

Thus, the occupation-number equation [Eq. (8)] becomes

$$\frac{\partial n_1(t)}{\partial t}=\frac{\pi}{\hbar}\sum_{234}\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)[(1-n_1)(1-n_2)n_3n_4-n_1n_2(1-n_3)(1-n_4)]|\langle1,2|v'|4,3-3,4\rangle|^2. \quad (15)$$

Together with Eq. (7), this equation completes our formulation of the ETDHF approximation. It describes properly the physics of the collision process and could have been written by taking note of energy conservation, Pauli principle, and transition probabilities.[12] Thus, Eq. (15) can be used not only in ETDHF but also in other microscopic non-self-consistent descriptions of collective dynamics.

With the Green's functions, corrections to the TDHF can be systematically introduced by considering Green's functions of higher and higher orders.[8,9] Furthermore, with the explicit determination of the collision matrix $I(x_1,x_1')$, macroscopic equations can be obtained in the usual way.[4] For example, one can show that the equation of continuity is preserved, that the total momentum is conserved, and that the total energy, which can be shown to be conserved, is split into the kinetic energy, the potential energy, and a new term which depends on particle collisions.

It is worth noting that under the constraint of $n_1=n_2$, $n_3=n_4$, and the constancy of the matrix element, we obtain an analytic solution of Eq. (15) when the "levels" $E_A=\epsilon_1+\epsilon_2$ and $E_B=\epsilon_3+\epsilon_4$ are linear functions of time and cross at $t=t_0$. The solution, which appears to be novel, can be easily shown to be

$$n_1(t)=\tfrac{1}{2}[(n_{10}+n_{30})+(n_{10}-n_{30})f(t)], \quad (16)$$

$$n_3(t)=\tfrac{1}{2}[(n_{10}+n_{30})-(n_{10}-n_{30})f(t)], \quad (17)$$

where

$$f(t)=\left\{\left[1+\left(\frac{Q_{20}}{a}\right)^2\right]\exp[\tfrac{1}{2}\pi a^2G^2\theta(t-t_0)-\left(\frac{Q_{20}}{a}\right)^2\right\}^{-1/2}, \quad (18)$$

$$Q_{20}=2(n_{10}-n_{30}), \quad a^2=8(n_{10}+n_{30})\left(1-\frac{n_{10}+n_{30}}{2}\right), \quad (19)$$

$$G^2=\frac{2}{\hbar}|\langle1,2|v'|4,3-3,4\rangle|^2\left|\frac{d}{dt}(E_A-E_B)\right|. \quad (20)$$

Here, the additional subscript 0 refers to values before the levels cross and $\theta(t-t_0)$ is the step function. This kind of level crossing is distinctly different from the usual Landau-Zener level crossing. For, if the rate $|d(E_A-E_B)/dt|$ is large, the occupation numbers are unchanged, as they should be, but, if the rate is small, the occupation probability is redistributed according to $n_1 \sim n_3 \sim \frac{1}{2}(n_{10}+n_{30})$. It is a redistribution such as the latter kind which brings an irregular distribution eventually to a Fermi-Dirac distribution characterized by a temperature.

It is easy to obtain many important results regarding thermal equilibrium and irreversibility. One defines an entropy s by

$$s=-k\sum_{\lambda}[n_\lambda \ln n_\lambda+(1-n_\lambda)\ln(1-n_\lambda)]. \tag{21}$$

One can prove easily the well-known H theorem that the entropy always increases,

$$\partial s(t)/\partial t \geq 0, \tag{22}$$

where the equality occurs at thermal equilibrium which is characterized by stationary occupation probabilities in the presence of particle collisions and corresponds to the vanishing of the collision matrix at all spatial points, achieved with a Fermi-Dirac distribution of occupation probabilities. In contrast, local equilibrium occurs when the collision matrix vanishes locally.

Approximation (11) makes use of only the expectation value of the single-particle Hamiltonian. There is, however, a spread of the single-particle strength because of particle collisions and the dynamics. If one assumes that each particle in a single-particle state has a lifetime, as in Landau Fermi-liquid theory,[12] then ϵ_i becomes $\epsilon_i - i\Gamma_i/2$. In consequence, the more general form of Eq. (15) is obtained by replacing the $\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ by the Lorentzian

$$\frac{\Gamma_{1234}}{2\pi[(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)^2+(\frac{1}{2}\Gamma_{1234})^2]},$$

and the step function $\theta(t-t_0)$ in Eq. (18) by

$$\frac{1}{\pi}\tan^{-1}\left(2\left|\frac{d}{dt}(E_A-E_B)\right|\frac{(t-t_0)}{\Gamma_{1234}}\right)+\frac{1}{2},$$

where $\Gamma_{1234}=\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4$. This introduction of a width allows the occupation numbers to change less abruptly and helps the numerical implementation of the ETDHF approximation.

To summarize, we have successfully extended the TDHF approximation to include particle collisions. The new formulation facilitates discussions of irreversible dissipation, thermal and local equilibrium, and hence hydrodynamical or nonhydrodynamical behavior of nuclear or other fermion fluids.

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