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THE INCORPORATION OF PARTICLE COLLISIONS IN THE TIME-DEPENDENT HARTREE-FOCK APPROXIMATION

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Abstract

In the time-dependent Hartree-Fock (TDHF) approximation, particles interact only through the mean field, and the collisions between particles are not included. Previously, we formulated the extended time-dependent Hartree-Fock (ETDHF) approximation to include particle collisions in terms of a temporal variation of the occupation probability n_λ for the single-particle states. In the simplest approximation, the single-particle potential is modified only through the particle density which depends on n_λ . We wish to refine the extended TDHF approximation by studying how particle collisions affect the single-particle potential. We find that it acquires two second-order contributions which are state-dependent and are the generalization of the "core polarization" and "correlation" contributions one encounters in the study of the nucleon-nucleus optical potentials. In consequence, concepts such as energy-dependent single-particle potentials and effective masses may be properly introduced in the extended TDHF approximation. We also wish to review the conservation of energy in the ETDHF approximation. We find that the total energy should include a second-order contribution due to correlations arising from particle collisions.

1. INTRODUCTION

In the time-dependent Hartree-Fock approximation, particles interact only through the mean field, and the collisions between particles are not taken into account.¹ It is a good description for many low-energy phenomena, where the Pauli exclusion principle inhibits collisions between particles. There are, however, problems in nuclear physics in which particle collisions are important. For example, in heavy-ion collisions much above a few MeV per nucleon, the Pauli exclusion principle is not effective in preventing particle collisions. In the problem of nucleon-nucleus reactions, the incident nucleon can excite nucleons in the nucleus from states below the Fermi energy to states above the Fermi energy. Particle collision is also very important in the search for a proper description for the approach to thermal equilibrium.^{2,3,6-9}

Previously, we formulated the extended time-dependent Hartree-Fock (ETDHF) approximation to incorporate particle collisions in the mean-field theory. Besides the temporal variation of the single-particle states, there is also a temporal variation of the occupation numbers n_λ governed by a master equation.^{2,3} Subsequent studies also lead to similar results.^{4,5} The collision term has also been examined from a random-matrix model,¹⁰ and the projection method.¹¹ Particle collisions are

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conjectured as possible agents of the iterative time-smoothing leading to dissipation in the time-dependent mean-field theory.¹² Other phenomenological ways to introduce the collision term have been presented.^{13,14} Numerical ETDHF calculations were performed for simple systems.¹⁵ The complete set of non-Markovian equations involving the one-body Green's function has been recently solved for non-equilibrium nuclear matter, with and without initial-state correlations.¹⁶

We wish to examine here other refinements of the ETDHF approximation. In the simplest approximation formulated so far, particle collisions affect the single-particle (SP) potential only through the particle density which depends on the occupation numbers. As is well known in nucleon-nucleus reactions, particle collisions give rise to polarization and correlation effects which lead to energy-dependent SP potentials.¹⁷⁻¹⁹ So, in the ETDHF approximation, one expects that particle collisions lead to second-order corrections of the SP potential in a similar manner.

Many questions have been raised about the conservation of energy in the ETDHF approximation.^{3-5,10,20} We shall review how the conservation of energy should be formulated and how the total energy should be defined in the presence of particle collisions.

II. EQUATION OF MOTION FOR THE GREEN'S FUNCTION

For a quantal many-body system, much of the dynamical information is contained in the Green's functions introduced by Martin and Schwinger.²¹ They are defined by

$$-i g^<(1 1') = \langle \hat{\psi}^+(1') \hat{\psi}(1) \rangle \quad (II.1)$$

$$i g^>(1 1') = \langle \hat{\psi}(1) \hat{\psi}^+(1') \rangle \quad (II.2)$$

where the expectation values of the field operators are taken with respect to the dynamical wave-packet-like state in question and the argument 1 (and similarly 1') represents the collection of space and spin coordinates x_1 and time coordinate t_1 . The Green's function $-ig^<(1 1')$ provide information about the occupation of single-particle states, while $ig^>(1 1')$ the non-occupancy of the single-particle states. The density matrix is the special equal-time case of the Green's function $g^<$.

We assume that the mean-field theory of TDHF, as obtained by using an effective density-dependent interaction $v(x_1 x_2) \delta(t_1 - t_2)$ and neglecting particle collisions, is a good and approximate representation of the dynamics. It is now necessary to include the residual interaction $v'(12) = v'(x_1 x_2) \delta(t_1 - t_2)$ between the fermions only in the Born scattering approximation. The equation of motion for $g^<$ in perturbation theory is²²

$$\left[i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1^2 - U_{HF}[\rho(1)] \right] g^<(1 1') \quad (II.3)$$

$$= \int_{-\infty}^{t_1} d\bar{T} \Sigma(1 \bar{T}) g^<(\bar{T} 1') - \int_{-\infty}^{t_1'} d\bar{T} \Sigma^<(1 \bar{T}) g(\bar{T} 1)$$

where $U_{HF}[\rho(1)]$ is the density-dependent single-particle potential obtained in the usual way.¹ The mass operators $\Sigma^>$ and $\Sigma^<$ are defined by

$$\Sigma^<(1 \bar{1}) = -i^2 \int d2 d\bar{2} v^<(1 2) v^<(\bar{1} \bar{2}) \mathcal{A}[g^<(1 \bar{1}) g^<(2 \bar{2})] g^<(\bar{2} 2), \quad (II.4)$$

where

$$\mathcal{A}[g^<(1 \bar{1}) g^<(2 \bar{2})] = g^<(1 \bar{1}) g^<(2 \bar{2}) - g^<(1 \bar{2}) g^<(2 \bar{1}).$$

The quantities Σ and g in Eq. (II.3) are

$$\Sigma(1 \bar{1}) = \Sigma^>(1 \bar{1}) - \Sigma^<(1 \bar{1}), \quad (II.5)$$

$$\text{and } g(1 \bar{1}) = g^>(1 \bar{1}) - g^<(1 \bar{1}). \quad (II.6)$$

The equation of motion for t_1' is

$$\left\{ -i \frac{\partial}{\partial t_1'} + \frac{\hbar^2}{2m} \nabla_1'^2 - U_{HF}[\rho(1')] \right\} g^<(1 1') \\ = \int_{-\infty}^{t_1} d\bar{1} g(1 \bar{1}) \Sigma^<(\bar{1} 1') - \int_{-\infty}^{t_1'} d\bar{1} g^<(1 \bar{1}) \Sigma(\bar{1} 1'). \quad (II.7)$$

Subtracting Eq. (II.7) from (II.3), we get the equation of motion for $g^<(1 1')$ from which kinetic equations can be derived:²²

$$\left\{ i\hbar \frac{\partial}{\partial t_1} + i\hbar \frac{\partial}{\partial t_1'} + \frac{\hbar^2}{2m} (\nabla_1^2 - \nabla_1'^2) - U_{HF}[\rho(1)] + U_{HF}[\rho(1')] \right\} g^<(1 1') \\ = \int_{-\infty}^t d\bar{1} \Sigma(1 \bar{1}) g^<(\bar{1} 1') - \int_{-\infty}^{t_1'} d\bar{1} \Sigma^<(1 \bar{1}) g(\bar{1} 1') \\ + \int_{-\infty}^{t_1'} d\bar{1} g^<(1 \bar{1}) \Sigma(\bar{1} 1') - \int_{-\infty}^{t_1} d\bar{1} g(1 \bar{1}) \Sigma^<(\bar{1} 1'). \quad (II.8)$$

III. EQUATIONS OF MOTION FOR ψ_λ AND n_λ

From the equations of motion for the Green's functions, we can derive the equations of motion for the single-particle states ψ_λ and the occupation probability n_λ by following the procedures presented previously.³ We specialize to an approximate representation of the Green's function in the form

$$-ig^<(1 1') = \sum_{\lambda} n_{\lambda}^<(t, t_1') \psi_{\lambda}(1) \psi_{\lambda}^*(1'), \quad (III.1)$$

$$\text{and } ig^>(1 1') = \sum_{\lambda} n_{\lambda}^>(t, t_1') \psi_{\lambda}(1) \psi_{\lambda}^*(1'), \quad (III.2)$$

where

$$n_{\lambda}^>(t, t_1) = 1 - n_{\lambda}^<(t_1 t_1). \quad (\text{III.3})$$

We also specialize to an approximate representation of the mass operator in the form

$$-i \Sigma^<(1 1') = \sum_{\lambda}^{\infty} \sigma_{\lambda}^<(t_1 t_1') \psi_{\lambda}(1) \psi_{\lambda}^*(1'), \quad (\text{III.4})$$

$$\text{and } i \Sigma^>(1 1') = \sum_{\lambda}^{\infty} \sigma_{\lambda}^>(t_1 t_1') \psi_{\lambda}(1) \psi_{\lambda}^*(1'). \quad (\text{III.5})$$

From Eq. (II.4), we can relate $\sigma^>$ with $n^>$ by

$$\sigma_{\lambda}^>(t_1 t_1') = \frac{1}{2} \sum_{234} n_3^>(t_1 t_1') n_4^>(t_1 t_1') n_2^<(t_1' t_1) \langle \lambda 2 | v' | 34 \rangle_{t_1} \langle 34 - 43 | v' | \lambda 2 \rangle_{t_1'} \quad (\text{III.6})$$

where the symbols 2, 3, and 4 stand for states λ_2 , λ_3 , and λ_4 , respectively, and the subscripts for the matrix elements specify the times at which the matrix elements are taken.

In order to have a Markovian equation of motion, it is necessary to parametrize the time dependence of $n_{\lambda}^>$ and $\langle 12 | v' | 34 \rangle_{t_1}$ in simpler forms so that the integration over history can be carried out. The quantity $n_{\lambda}^<(t_1 t_1')$ is the probability that a particle at state λ is destroyed at time t_1 and emerges at time t_1' . Anticipating the results of the master equation, we know that a particle or a hole has a lifetime and decays exponentially³ as $\exp(-\Gamma_{\lambda}^c t/\hbar)$. It is reasonable to parametrize $n^<$ and $n^>$ by

$$n_{\lambda}^>(t_1 t_1') = n_{\lambda}^>(T) e^{-\Gamma_{\lambda}^c |t_1' - t_1|/2} \quad (\text{III.7})$$

where $T = (t_1 + t_1')/2$ and Γ_{λ}^c is [see Eqs. (9.11)-(9.17) of Ref. 3]

$$\Gamma_{\lambda}^c = \hbar(P_{\lambda}^{(-)} + P_{\lambda}^{(+)}), \quad (\text{III.8})$$

with $P^{(-)}$ and $P^{(+)}$ defined by the master equation

$$\frac{\partial n_{\lambda}^<(T)}{\partial T} = -P_{\lambda}^{(-)} n_{\lambda}^< + P_{\lambda}^{(+)} (1 - n_{\lambda}^<). \quad (\text{III.9})$$

The superscript c for the width denotes that it arises from particle collisions.

To parametrize the time-dependence of the matrix element $\langle \lambda 2 | v' | 34 \rangle$, we note that the overlap of the single-particle state ψ_{λ} at two different times is

$$\langle \psi_{\lambda}(t_1) | \psi_{\lambda}(t_1') \rangle \approx \exp \left\{ -i \int_{t_1}^{t_1'} \epsilon_{\lambda}(t') dt' - \frac{1}{2} [D_{\lambda}(T)]^2 (t_1' - t_1)^2 \right\} \quad (\text{III.10})$$

where

$$\epsilon_\lambda(t) = (\psi_\lambda(t), h \psi_\lambda(t)), \quad (\text{III.11})$$

h is the single-particle hamiltonian, and D_λ is the second moment of h defined by

$$D_\lambda^2(T) = (\psi_\lambda(T), [h - \epsilon_\lambda(T)]^2 \psi_\lambda(T)). \quad (\text{III.12})$$

It is more convenient to work with the factor $\exp(-\Gamma|t_1' - t_1|/2)$ than with the Gaussian factor in time. We approximate Eq. (III.10) by

$$\langle \psi_\lambda(t_1) | \psi_\lambda(t_1') \rangle \simeq e^{-i \epsilon_\lambda(T)(t_1' - t_1) - \Gamma_\lambda^d(T)|t_1' - t_1|/2} \quad (\text{III.13})$$

where

$$\Gamma_\lambda^d = 2(8/\pi)^{1/6} D_\lambda, \quad (\text{III.14})$$

chosen in such a way that the two factors have the same second moments. The superscript d denotes that the width arises from the dynamical motion of the nucleons.³ The dynamical width was also discussed in Refs. 10 and 20.

Equation (III.13) suggests that it is reasonable to approximate the time-dependence of the matrix element by

$$\langle \lambda 2 | v^\dagger \beta 4 \rangle_{t_1} \simeq e^{-i \epsilon(t_1 - T) - \Gamma^d |t_1 - T|/2} \langle \lambda 2 | v^\dagger \beta 4 \rangle_T, \quad (\text{III.15})$$

where

$$\epsilon = \epsilon_3 + \epsilon_4 - \epsilon_\lambda - \epsilon_2, \quad (\text{III.16})$$

$$\text{and } \Gamma^d = \Gamma_\lambda^d + \Gamma_2^d + \Gamma_3^d + \Gamma_4^d. \quad (\text{III.17})$$

For a slowly varying mean field, the integration over time can now be carried out in Eq. (II.8) for $t_1' = t_1^+$. After taking the scalar product of Eq. (II.8) with respect to $\psi_\lambda(1)\psi_\lambda^*(1')$ and integrating over $\bar{t}_1$, we separate out an equation for t_1 and another equation for t_1' . In this separation, we ascribe half of the second term and half of the fourth term of the righthand side of Eq. (II.8) to each of these two equations. The resultant equation in t_1 reads

$$\begin{aligned}
& (\psi_\lambda(1), \left[i \frac{\partial}{\partial t_1} + \frac{\hbar^2 \nabla^2}{2m} - U_{HF}(1) \right] n_\lambda^\zeta(t_1 t_1^\dagger) \psi_\lambda(1)) \\
& = -\frac{1}{2} \sum_{234} [n_3^\zeta n_4^\zeta n_2^\zeta + n_3^\zeta n_4^\zeta n_2^\zeta] n_\lambda^\zeta \frac{\epsilon}{\epsilon^2 + (\Gamma/2)^2} \left| \langle 12 | v^- | 34-43 \rangle_{t_1} \right|^2 \\
& + \frac{1}{2} \sum_{234} [n_3^\zeta n_4^\zeta n_2^\zeta n_\lambda^\zeta - n_3^\zeta n_4^\zeta n_\lambda^\zeta n_2^\zeta] \frac{i \Gamma/2}{\epsilon^2 + (\Gamma/2)^2} \left| \langle 12 | v^- | 34-43 \rangle_{t_1} \right|^2
\end{aligned} \quad (III.18)$$

where

$$\Gamma = \Gamma^C + \Gamma^d = (\Gamma_\lambda^C + \Gamma_2^C + \Gamma_3^C + \Gamma_4^C) + \Gamma^d. \quad (III.19)$$

The equation for $t_1^\dagger$ is just the complex conjugation of Eq. (III.18). Separating out the real and imaginary parts of these equations, we get the master equation

$$\begin{aligned}
\frac{\partial n_\lambda^\zeta(T)}{\partial T} &= \sum_{234} [n_3^\zeta(T) n_4^\zeta(T) n_\lambda^\zeta(T) n_2^\zeta(T) - n_3^\zeta(T) n_4^\zeta(T) n_\lambda^\zeta(T) n_2^\zeta(T)] \\
&\times \frac{\Gamma/2}{\epsilon^2 + (\Gamma/2)^2} \left| \langle 12 | v^- | 34-43 \rangle_T \right|^2
\end{aligned} \quad (III.20)$$

and the single-particle equation

$$\left[i \hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1^2 - U_{HF}(1) - \Delta U_\lambda \right] \psi_\lambda(1) = 0 \quad (III.21)$$

where

$$\Delta U_\lambda \psi_\lambda(1) = - \sum_{234} [n_3^\zeta n_4^\zeta n_2^\zeta + n_3^\zeta n_4^\zeta n_2^\zeta] \frac{\epsilon}{\epsilon^2 + (\Gamma/2)^2} \langle 34-43 | v^- | 12 \rangle_{t_1} \quad (III.22)$$

$$\int dx_2 \psi_2^*(x_2) v^-(x_1 x_2) \psi_4(x_2) \psi_3(x_1).$$

The potential ΔU_λ is spatially non-local and state-dependent. An approximate representation of $\Delta U_\lambda \psi_\lambda(1)$ is

$$\Delta U_\lambda \psi_\lambda(1) \sim - \frac{1}{2} \sum_{234} [n_3^\zeta n_4^\zeta n_2^\zeta + n_3^\zeta n_4^\zeta n_2^\zeta] \frac{\epsilon}{\epsilon^2 + (\Gamma/2)^2} \left| \langle 12 | v^- | 34-43 \rangle_{t_1} \right|^2 \psi_\lambda(1) \quad (III.23)$$

Equation (III.20) is the same as what was derived earlier. The SP potential in Eq. (III.21) acquires two new second-order terms which are analogous to the polarization and correlation terms one encounters in the theory of nucleon-nucleus optical-model

potentials¹⁷⁻¹⁹ [cf. Eqs. (2.159-2.160) of Ref. 18]. They have the same physical origin as in the optical potential case and lead to a non-local and energy-dependent SP potential. The two contributions have a tendency to have opposite signs. As in the nucleon-nucleus case, the SP potential may be described in terms of an energy-dependent effective mass m^* . It is known that the effective mass m^* of a nucleon is about the nucleon mass m at ϵ_f but decreases to about $0.7m$ for $\epsilon_\lambda \sim \epsilon_f + 2\hbar\omega$.^{18,19} So, one should use an effective mass of about $0.7m$ for heavy-ion reactions with energy greater than 10 MeV per nucleon.

IV. CONSERVATION OF ENERGY IN THE ETDHF APPROXIMATION

There have been many questions raised concerning the conservation of energy in the ETDHF approximation. At the root of the problem is the confusion as to how the total energy quantity should be defined so that it is conserved as a function of time. Clearly, the additional degree of freedom introduced by the particle collisions requires that there is an energy contribution arising from this degree of freedom. Energy quantities calculated without this correlation will not, in general, be conserved.

Kadanoff and Baym obtained the conservation laws in the perturbation theory.²² In particular, when the Born scattering term is considered, the total energy defined in the following way is a conserved quantity:

$$E_{\text{tot}} = \int dx_1 T(x_1) + (i^2/2) \int dx_1 dx_2 v(x_1 x_2) g_2(12, 1^+ 2^+) \quad (\text{IV.1})$$

where $T(x_1)$ is the kinetic energy density

$$T(x_1) = \frac{\hbar^2}{2im} \lim_{1' \rightarrow 1} \nabla_1 \cdot \nabla_{1'} g^<(1, 1'), \quad (\text{IV.2})$$

$$g_2(12, 1^+ 2^+) = \cancel{A} [g^<(1 \ 1^+) g^<(2 \ 2^+)] + g_{2c}(12, 1^+ 2^+), \quad (\text{IV.3})$$

and in the Born scattering approximation

$$g_{2c}(12, 1^+ 2^+) = \frac{i}{\hbar} \int d\bar{1} d\bar{2} v(\bar{1} \ \bar{2}) \int_{-\infty}^{t_1} d\bar{t} \left\{ g^>(1 \ \bar{1}) g^>(2 \ \bar{2}) \cancel{A} [g^<(\bar{1} \ 1^-) g^<(\bar{2} \ 2^-)] \right. \\ \left. - g^<(1 \ \bar{1}) g^<(2 \ \bar{2}) \cancel{A} [g^>(\bar{1} \ 1^-) g^>(\bar{2} \ 2^-)] \right\}. \quad (\text{IV.4})$$

For a system where the effective mean-field interaction is different from the effective residual interaction, the total energy is modified to be³

$$E_{\text{tot}} = \int dx_1 T(x_1) + \frac{i^2}{2} \int dx_1 dx_2 v(x_1 x_2) \Delta [g^<(1^+ 1^+) g^<(2^+ 2^+)] \\ + \frac{i^2}{2} \int dx_1 dx_2 v^-(x_1 x_2) g_{2c}(12, 1^+ 2^+). \quad (\text{IV.5})$$

The first two terms give the Hartree-Fock energy E_{HF} , while the last term is the energy due to correlations arising from particle collisions. With the parametrization of the Green's function as given previously, we find that for slowly varying mean field, the total energy is

$$E_{\text{tot}} = E_{\text{HF}} + E_{\text{coll}} \quad (\text{IV.6})$$

where

$$E_{\text{coll}} = \frac{1}{4} \sum_{\lambda 234} \left| \langle \lambda 2 | v^- | 34 \rangle \right|^2 \left[n_{\lambda}^< n_2^< n_3^> n_4^> - n_{\lambda}^> n_2^> n_3^< n_4^< \right] \frac{\epsilon}{\epsilon^2 + (\Gamma/2)^2}. \quad (\text{IV.7})$$

The energy E_{coll} due to particle collisions contains two contributions which have a tendency to have the same positive signs. The quantity E_{tot} is conserved if the slowly varying mean field is a good approximation.

V. DISCUSSION

We have considered two of the outstanding problems in the ETDHF approximation. We found that particle collisions off the energy shell contribute to non-local state-dependent corrections to the mean field. In the form of the approximation Eq. (III.23), these corrections correspond to a shift in the single-particle energy. The shift is small for states near the Fermi energy, large and negative for deep-hole states, and large and positive for high-lying particle states.¹⁸ In the optical model, the energy dependence in the potential is an important consideration. It should also be an important factor in the discussion of heavy-ion collisions.

With regard to the question of energy conservation, a total energy quantity including the contributions from particle collision is conserved if the mean-field varies slowly. It is an approximately conserved quantity when the mean field varies rapidly. Energy quantities calculated with only the Hartree-Fock approximation are not conserved in the presence of particle collisions.

There remains an unresolved problem which deserves attention. As it is presented, the ETDHF approximation depends on the choice of basis states. This need not be the case but is a simplification which makes the problem tractable. For example, instead of working with the occupation probability $n_{\lambda}(t_1 t_1')$, one can introduce an occupation matrix $n_{\lambda\lambda'}(t_1 t_1')$ to represent the Green's function. The results will be basis-independent, but the equation of motion involves a seven-fold sum over the state indices (see Appendix B of Ref. 3). The complexity of the numerical problem becomes enormous. The use of the occupation probability n_{λ} instead of the matrix

$n_{\lambda\lambda'}$ relies on a choice of good basis states in terms of which the dynamics of the simplified problem approximates reasonably well the dynamics of the full, but complicated, problem. It is important to avoid forbidding transitions which would otherwise be allowed in the full problem. We can therefore judge that the choice of the basis states in the center-of-mass system is not a good one. For, in the simplified problem with n_{λ} , a state is characterized by the expectation value of h . For the collision of two equal nuclei, the single-particle states for the left nucleus and the right nucleus will be initially degenerate. There is a complete overlap of the n_{λ} distribution for the two nuclei. In contrast, in the full problem with $n_{\lambda\lambda'}$, the off-diagonal matrix element provides an extra degree of freedom so that, even though the two distributions overlap in the energy space, it does not completely overlap in the other degrees of freedom. The degree of having no overlap increases with energy, and opens up a larger phase space for particle collisions. To mimic this separation between the two distributions in our simplified problem with our limited degree of freedom, we are well advised to use a coordinate system in which one of the nuclei (say, the heavier one) is at rest. In such a case, occupied states in one nucleus can make transitions to unoccupied states in the other nucleus more readily. Previous ETDHF calculations were performed in the center-of-mass system.¹⁵ It will be of interest to repeat the calculations for the laboratory system and see how particle collisions may affect the λ -window. Clearly, future theoretical investigations on the choice of the best basis states will be of great interest.

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