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# Dynamics of nuclear fluid. V. Extended time-dependent Hartree-Fock approximation illuminates the approach to thermal equilibrium

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In the time-dependent Hartree-Fock approximation, the fermions are assumed to interact only through the mean field and the collisions between particles are neglected. We formulate an extended time-dependent Hartree-Fock approximation which incorporates particle collisions due to the residual interaction, with the usual time-dependent Hartree-Fock approximation as the collisionless limit. It is obtained by a truncation of the Martin-Schwinger hierarchy at the second level and by using a simple representation of the one-body Green's function in terms of time-dependent occupation numbers. The final set of coupled equations consists of a modified time-dependent Hartree-Fock equation and a master equation for the occupation numbers. These results are physically transparent and describe properly the physics of the collision process. They may also be simple enough to be of practical use to study heavy-ion collisions or the dynamics of other fermion systems. Furthermore, as the configuration-space analog of the quantum Boltzmann equation, many important results concerning statistical dynamics are obtained. Concepts such as entropy, temperature, and local and thermal equilibrium can be quantitatively introduced. The well-known *H* theorem that entropy never decreases can be readily recovered. With the collision term explicitly exhibited, the macroscopic equations (equations of continuity, momentum flux, and energy) and their associated conservation theorems can also be derived. Analytic solutions for the master equation for simple cases lead to new "level crossing" formulas having characteristics distinctly different from the Landau-Zener level-crossing formula and illuminate the salient features as to how a nonequilibrium fermion system approaches thermal equilibrium.

[NUCLEAR REACTIONS Extension of time-dependent Hartree-Fock approximation. Collisions between particles. Master equation for occupation probabilities. Entropy, temperature, and thermal equilibrium. *H* theorem. Analytic solution of the master equation. New types of level crossing formula.]

## I. INTRODUCTION

This is the fifth of a series of articles dealing with the dynamics of nuclear fluid. Other studies concern themselves with the equations governing the dynamics starting with time-dependent Hartree-Fock approximations (TDHF),[1] the generalization of the time-dependent Hartree-Fock approximation to include spin and isospin degrees of freedom,[2] the kinetic theory of quantum fluids,[3] and spin and isospin properties of finite nuclei in the hydrodynamical model.[4] We present here an extension of the TDHF approximation and the consequences of such an extension on the dynamics of the nuclear fluid. A brief summary of the main results has been reported previously.[5] Independent but later investigations[6-8] along similar lines have also been carried out by Shakin and Weiss[6] and also by Orland and Schaeffer[7] leading to similar results for the extended time-dependent Hartree-Fock approximation.

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.[9] Since then, many TDHF calculations were carried out[9-12] and many different theoretical investigations were initiated.[13-19,1-7] 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 energy and momentum states of the colliding particles and dissipating energies, the pattern of behavior of the quantum fluid can be that of hydrodynamics[3] or elastic response,[17,18,3] depending on the degree of particle collisions. Because of such dependence, it is of interest to extend the TDHF approximation to include particle collisions.

A previous extension of the time-dependent Hartree-Fock approximation was discussed in terms of a multideterminant representation and Pauli's master equation.[3] However, the use of a multideterminantal wave function is unsatisfactory in that, in a channel coupling sense, the number of determinants one can couple in a practical multideterminant TDHF calculation is rather limited. There is also the associated difficulty of extracting statistical dynamical information from a limited set of determinants. It is desirable to seek a different extension of the time-dependent Hartree-Fock approximation.

Although the TDHF equations can be derived from a variational principle,[20-22] it is well known that it can be viewed as the lowest truncation of a hierarchy of coupled equations.[23,24,1,3] The fact that one has high expectations that even the lowest truncation can give a good representation of the dynamics relies on the introduction of effective interactions for which much of the higher-order correlations have been, in principle, incorporated. What has not been incorporated is the dynamical correlation due to particle collisions. From this viewpoint, a natural extension of the TDHF approximation can be obtained by truncating the hierarchy at a higher level.

There are two hierarchies in which the TDHF approximation appears as the simplest truncation. In terms of the density matrices, there is the hierarchy of the quantum kinetic equations of Bogoliubov and Gurov,[25] and Born and Green[26] coupling the one-body density to the two-body density matrix which in turn is coupled to the three-body density matrix.[3] It is the quantum analog of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy in classical many-body problems.[26-29] On the other hand, in terms of the Green's functions, there is the Martin-Schwinger hierarchy[23] coupling the one-body Green's function to the two-body Green's function which in turn is coupled to the three-body Green's function. Because density matrix is a special equal-time Green's function, the Martin-Schwinger hierarchy contains the quantum BBGKY hierarchy as a special case and is therefore a larger and more general set. The possibility of manipulating Green's functions with unequal time coordinates makes the Martin-Schwinger hierachy well adapted to discuss transport phenomena. The success of deriving the Uehling-Uhlenbeck[30] equation for an infinite medium using the Martin-Schwinger hierarchy by Kadanoff and Baym[24] suggests the fruitfulness of a similar approach for finite nuclei which we shall follow. As the TDHF single-particle equations are usually solved in the configuration space, we wish to limit our consideration to that space in preference to the Wigner space where much progress in obtaining the kinetic equation for normal quantum fluid has been made recently.[31]

We wish to obtain a set of final equations for our finite nuclear systems as the configuration-space analog of the quantum Boltzmann equation. Consequently, this set of equations should retain certain characteristics of the Boltzmann equation. It should be Markovian in the sense that all the quantities are to be specified at the same time coordinate.[32] 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. This means that it suffices to include only the Born collision term in the perturbation expansion of the Green's function. Finally, as the Boltzmann equation violates time-reversal invariance, we would like to take note of the time-reversal violation when it is introduced.

By truncating the Martin-Schwinger hierarchy at the second level and using simple representations of the one-body Green's functions in terms of time-dependent occupation numbers of modified time-dependent Hartree-Fock single-particle basis states, we obtain a final set of equations which consists of an equation defining the basis states and a master equation for the occupation numbers. The equation for the single-particle states is a "modified" TDHF equation in the sense that the density which appears in the self-consistent potential now depends on the time-dependent occupation numbers. The master equation for the occupation number is simple and physically transparent. It could have been written down directly by taking note of energy conservation, Pauli principle, and transition probabilities. Nevertheless, the Green's function method adopted here has the advantage that higher-order corrections to the TDHF approximation can be systematically introduced if one so desires.

To obtain a generalization of the TDHF approximation and indicating how corrections can be introduced systematically is not the only purpose of the present investigation. Knowing the kinetic equations, one has a powerful tool to study transport phenomena and the approach to equilibrium. Although much progress has been made recently concerning dissipative phenomena in nuclear systems,[33-35] many important questions remain unanswered. For example, one may wish to know how a nuclear system (either in a heavy-ion collision or in the vibration of a single nucleus) does or does not equilibrate, and if it does equilibrate, how a temperature is acquired. One may also wish to know whether concepts such as entropy, temperature, thermal equilibrium, local equilibrium, valid enough for macroscropic systems, can be quantitatively introduced for finite nuclear systems, and if so, how one can prove that entropy never decreases. These and related questions can be discussed with our final set of equations for the extended time-dependent Hartree-Fock (ETDHF) approximation. In the process, we obtain analytic solutions of the master equation. These solutions give rise to new "level-crossing" formulas having characteristics quite distinctly different from the Landau-Zener level crossing and illuminate the salient features as to how a nonequilibrium fermion system approaches equilibrium.

Our results are useful also in a different context. Previously, from the TDHF approximation, we wrote down the equations of motion for the macroscopic variables which are what one obtains in classical inviscid hydrodynamics with the exception of the presence of terms of quantum origin.[1,2,3,4,19] Our formulation of the collision term paves the way for a better connection between the microscopic description and the macroscopic description involving irreversible dissipation.

This paper is organized as follows. In Sec. II, we introduce the Martin-Schwinger hierarchy and show how the lowest truncation obtained by neglecting the correlated part of the two-body Green's function $g_{2c}$ due to particle collision leads to the time-dependent Hartree-Fock approximation. Thus, a natural extension of the time-dependent Hartree-Fock approximation is obtained if one includes the correlated part $g_{2c}$. In Sec. III, we go to the next level of the hierarchy to obtain an equation of motion for $g_{2c}$. In the Born approximation, this equation can be solved to obtain $g_{2c}$ in terms of the one-body Green's function. The resultant equation of motion for the one-body Green's function is, however, non-Markovian in the sense that it contains not only the Green's function at the present time under consideration, but also the Green's function over the past collision history. In order to obtain a Markovian equation of motion, we first specialize in Sec. IV to a simple representation of the Green's function in terms of time-dependent occupation numbers in a complete set of "modified" TDHF basis states. Such a choice leads to a clean separation between the effects due to the mean field and the effects due to particle collisions. Next, in Sec. V, we limit our attention to slowly varying mean fields such that simplifying assumptions can be made concerning the temperal behavior of some of the quantities. These simplifying assumptions allow one to evaluate the correlated part of the two-body Green's function $g_{2c}$ in terms of quantities defined at the same time coordinate. A master equation for the occupation number is obtained to complete the formulation of the ETDHF approximation and forms the basis of investigation in the subsequent sections.

The consequences of the ETDHF approximation is explored in Secs. VI to XII. Before such an exploration, we summarize the resultant equations of the ETDHF equation and indicate possible refinements in Sec. VI. Analytic solutions of the master equation are obtained for four isolated states in Sec. VII. These solutions have features distinctly different from the Landau-Zener level-crossing formula. In Sec. VIII, we introduce the entropy and prove the well-known theorem that the entropy never decreases. A scenario on how a finite nucleus approaches thermal equilibrium is presented by making use of the features of the solutions of the master equation obtained in Sec. VII. In Sec. IX, we investigate the properties of the static self-consistent equilibrium solutions in the presence of particle collision. In Secs. X and XI, the macroscopic equations and their associated conservation theorems are derived to make a connection between microscopic descriptions in the ETDHF approximations with the macroscopic descriptions in terms of density, velocity, and kinetic energy density. The many-body information extracted from ETDHF approximation is investigated in Sec. XII. Section XIII summarizes the present discussion.

As one can see, this paper consists of two main parts. Namely, Secs. II to V deal with the derivation of the extended time-dependent Hartree-Fock approximation, while the remaining sections are concerned with the resultant statistical dynamical information extracted therefrom. Each part is more or less self-contained. Thus, if one is interested mainly in the consequences and applications of the ETDHF approximation, one can satisfy oneself that the final set of equations of the ETDHF approximation describes properly the physics of the process with regard to Pauli principle and transition probabilities and can go directly to Sec. VI for a summary of the ETDHF approximation. One can then proceed to the next few sections to see how it can be used to study irreversible dissipative phenomena in nuclear dynamics.

In this paper three appendices are provided to clarify some of the points discussed in the main text. In Appendix A, the equivalence of the TDHF approximation in density matrix form and the TDHF approximation in terms of single-particle equations are investigated from a rigorous mathematical viewpoint. In Appendix B, we write down the master equation for the more general (but less practical) case when the Green's function is represented in terms of an occupation number matrix $n_{\lambda\lambda'}$, instead of an occupation number $n_\lambda (= n_{\lambda\lambda})$. The complexity of the problem is indicated by the presence of a sevenfold summation in the master equation. In Appendix C, for practical purposes, we exhibit the master equation for the occupation numbers when the spin and isospin degrees of freedom are averaged over.

## II. THE FIRST EQUATION OF THE MARTIN-SCHWINGER HIERARCHY

For a quantal many-body system, much of the detailed dynamical information and possible information about the statistical mechanics of the system are contained in the Green's function introduced by Martin and Schwinger.[23] A comprehensive review of the formalism is given by Kadanoff and Baym[24] and also by Abrikosov, Gorkov, and Dzyaloshinski.[36] We shall briefly summarize the pertinent results of Martin and Schwinger as the starting point of our investigation.

In the Heisenberg representation, the Hamiltonian for a system of nucleons of mass $m$ interacting through an instantaneous two-body potential $v(x_1, x_2')$ is given by

$$H = \frac{\hbar^2}{2m} \int dx \nabla \hat{\psi}^\dagger(x,t) \cdot \nabla \hat{\psi}(x,t) + \tfrac{1}{2} \int dx dx' \hat{\psi}^\dagger(x,t) \hat{\psi}^\dagger(x',t) v(x,x') \times \hat{\psi}(x',t) \hat{\psi}(x,t) \,, \tag{2.1}$$

where $x$ represents the collection of the spatial coordinate $\vec{\mathrm{r}}$, the spin, and isospin coordinate $\xi$. The equation of motion for the field operator $\hat{\psi}$ is therefore

$$\left(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \nabla^2}{2m}\right) \hat{\psi}(x,t) = \int dx' v(x,x') \hat{\psi}^\dagger(x',t) \hat{\psi}(x',t) \hat{\psi}(x,t) \,. \tag{2.2}$$

By multiplying the above equation on the left by $\hat{\psi}^\dagger(x',t')$ and taking the expectation value of the time-ordered product, we obtain

$$\left(i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1{}^2\right) g(1,1') = \hbar \delta(1-1') + (-i) \int d2 v(1,2) g_2(12, 1'2^+) \,, \tag{2.3}$$

where the symbol 1 (and analogously 1′, 2, and $2^+$) represents the collection of coordinates $x_1$ and $t_1$. The Green's functions are defined by

$$g(1,1') = (-i) \langle T(\hat{\psi}(1) \hat{\psi}^\dagger(1')) \rangle \tag{2.4}$$

and

$$g_2(12, 1'2') = (-i)^2 \langle T(\hat{\psi}(1) \hat{\psi}(2) \hat{\psi}^\dagger(2') \hat{\psi}^\dagger(1')) \rangle \,, \tag{2.5}$$

the expectation value of the time-ordered product being taken with respect to the dynamical wave-packet-like state in question. We have also used the symbol $v(1,2)$ to represent $v(x_1, x_2)\delta(t_1 - t_2)$ and the symbol $2^+$ to imply that the time coordinate $t_2^+$ here is greater than, but approaches $t_2$ in the limit.

Equation (2.3), the first of the Martin-Schwinger hierarchy of equations, couples the one-body Green's function to the two-body Green's function. The two-body Green's function is, in turn, coupled to the three-body Green's function. This kind of coupling continues on to form a hierarchy of coupled equations for the many-body Green's functions.

It is instructive to show that the time-dependent Hartree-Fock approximation can be obtained as simplest truncation of the hierarchy. For this purpose, it is convenient to introduce the Green's function $g^<$ and $g^>$ as[23,24]

$$ig^<(1,1') = - \langle \hat{\psi}^\dagger(1') \hat{\psi}(1) \rangle \tag{2.6}$$

and

$$ig^>(1,1') = \langle \hat{\psi}(1) \psi^\dagger(1') \rangle \,, \tag{2.7}$$

so that

$$g(1,1') = g^<(1,1') \text{ if } t_1 < t_1' \tag{2.8}$$

and

$$g(1,1') = g^>(1,1') \text{ if } t_1 > t_1' \,. \tag{2.9}$$

For our application, it is sufficient to limit our attention to the case where $t_1'$ is greater than $t_1$ but approaches $t_1$ in the limit. We separate the two-body Green's function into a free uncorrelated (Hartree-Fock) part $g_{20}$ and a correlated part $g_{2c}$ due to particle collisions:

$$g_2(12, 1'2^+) = g_{20}(12, 1'2^+) + g_{2c}(12, 1'2^+) \,, \tag{2.10}$$

where

$$g_{20}(12, 1'2^+) \equiv \mathcal{A}[g^<(1,1') g^<(2,2^+)] \tag{2.11}$$

$$= g^<(1,1') g^<(2,2^+) - g^<(1,2^+) g^<(2,1') \,, \tag{2.12}$$

and the operator $\mathcal{A}$ is the antisymmetrization operator. Thus, Eq. (2.3) can be written in the following form:

$$\left(i\hbar \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1{}^2 - U_{\mathrm{MHF}}(1)\right) g^<(1,1') = \hbar \delta(1-1') + (-i) \int d2 v(1,2) g_{2c}(12, 1'2^+) \,, \tag{2.13}$$

where the modified Hartree-Fock potential $U_{\mathrm{MHF}}(1)$ is defined by

$$U_{\mathrm{MHF}}(1)g^{<}(1,1')=(-i)\int d2\,v(1,2)\mathcal{A}[g^{<}(1,1')g^{<}(2,2^{+})]\,. \tag{2.14}$$

(We use the "modified" to indicate that as distinct from the Hartree-Fock case, here, the equal-time Green's function is not necessarily determined by a single determinantal wave function.)

From Eq. (2.13) and its adjoint equation of motion, we obtain

$$\left(i\hbar\frac{\partial}{\partial t_1}+i\hbar\frac{\partial}{\partial t_1'}+\frac{\hbar^2}{2m}(\nabla_1{}^2-\nabla_{1'}{}^2)-U_{\mathrm{MHF}}(1)+U_{\mathrm{MHF}}(1')\right)g^{<}(1,1')=I(1,1')\,, \tag{2.15}$$

where the collision matrix $I(1,1')$ is defined for $t_1'=t_1^{+}$ as

$$I(x_1t_1,x_1't_1^{+})=(-i)\int dx_2[v(x_1,x_2)-v(x_1',x_2)]g_{2c}(12,1'2^{+})\Big|_{\substack{t_1'=t_1^{+}\\ t_1=t_2}}\,. \tag{2.16}$$

The correspondence between the time-dependent Hartree-Fock equation and Eq. (2.15) obtained from the first equation of the Martin-Schwinger hierarchy can be readily recognized. One notes that the equal-time one-body Green's function $g^{<}$ is just the density matrix:

$$\lim_{t_1'\to t_1}[-ig^{<}(x_1,t_1,x_1',t_1')]=\mathfrak{N}(x_1,x_1';t_1)\,. \tag{2.17}$$

Thus, when the collision matrix $I(1,1')$ is neglected, Eq. (2.15) becomes the time-dependent Hartree-Fock equation

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\mathfrak{N}(x_1,x_1';t)=&-\frac{\hbar^2}{2m}(\nabla_1{}^2-\nabla_{1'}{}^2)\mathfrak{N}(x_1,x_1';t)\\ &+\int dx_2[v(x_1,x_2)-v(x_1',x_2)][\mathfrak{N}(x_1,x_1';t)\mathfrak{N}(x_2,x_2;t)-\mathfrak{N}(x_1,x_2;t)\mathfrak{N}(x_2,x_1';t)]\,. \end{aligned} \tag{2.18}$$

The use of the idempotent property, symmetry, and finite normalization conditions then leads one from the TDHF equation in density matrix form to the TDHF equation in single-particle equation form (Appendix A).

The recognition that the TDHF is the simplest truncation of the Martin-Schwinger hierarchy is useful not only as a way to understand how TDHF equations can be derived, such a recognition also allows one to find the corrections to the TDHF approximation. Obviously, the inclusion of the collision matrix will provide the next correction to the TDHF approximation. For the evaluation of the collision matrix, it is necessary to go to the next level of the Martin-Schwinger hierarchy.

## III. THE SECOND EQUATION OF THE MARTIN-SCHWINGER HIERARCHY

For a quantum system in a canonical ensemble of thermal equilibrium, the two-body Green's function can be obtained as an expansion in powers of the interaction.[23,24,36] Diagrammatic rules for writing down the perturbation expansion have been well developed using the field theoretical technique.[36] For our case under consideration, we do not have a canonical ensemble, but a wave-packet-like dynamical nonequilibrium state; the final result of perturbation expansion of the two-body Green's function remains the same[37-40] except that the path of time integration and the ordering of the field operators need to be defined in a more general way. We shall obtain the perturbation expansion using these diagrammatic rules. As we mentioned before, in analogy with the classical Boltzmann equation, we need to include only the Born collision term in the perturbation expansion of the Green's function. For such a simple case, the structure of the perturbation expansion can be obtained by considering the second equation of the Martin-Schwinger hierarchy. However, it is still necessary to return to the field theoretical method for perturbation expansion of the Green's functions in the real-time domain[37-40] in order to define properly the time-integration path and the ordering of the field operators. In spite of such a limitation, it is nonetheless instructive to study how the Born collision term can be obtained from the Martin-Schwinger hierarchy. The first two equations in the hierarchy are of the form

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\nabla_1{}^2\right)g(1,1')=\hbar\delta(1-1')+(-i)\int d2\,v(1,2)g_2(12,1'2^{+})\,, \tag{3.1}$$

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\nabla_1{}^2\right)g_2(12,1'2')=\hbar[\delta(1-1')g(2,2')-\delta(1-2')g(2,1')]+(-i)\int d3v(1,3)g_3(123,1'2'3^+)\,. \tag{3.2}$$

A truncation is achieved by assuming a product form of the three-body Green's function

$$g_3(123,1'2'3^+)\simeq\mathcal{A}[g_2(12,1'2')g(3,3^+)]\,, \tag{3.3}$$

where

$$\mathcal{A}[g_2(12,1'2')g(3,3^+)]=g_2(12,1'2')g(3,3^+)-g_2(12,3^+2')g(3,1')-g_2(12,1'3^+)g(3,2')\,, \tag{3.4}$$

which leads to

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\nabla_1{}^2-U_{\mathrm{MHF}}(1)\right)\left(i\hbar\frac{\partial}{\partial t_2}+\frac{\hbar^2}{2m}\nabla_2{}^2-U_{\mathrm{MHF}}(2)\right)\{g_2(12,1'2')-\mathcal{A}[g(1,1')g(2,2')]\}=i\hbar v(1,2)g_2(12,1'2')+O(v^2)\,. \tag{3.5}$$

To the first order in $v$, the correlated part of the two-body Green's function is

$$g_2(12,1'2')-\mathcal{A}[g(1,1')g(2,2')]=\frac{i}{\hbar}\int d\bar{1}d\bar{2}g(1,\bar{1})g(2,\bar{2})v(\bar{1},\bar{2})\mathcal{A}[g(\bar{1},1')g(\bar{2},2')]\,, \tag{3.6}$$

which is the perturbation expansion result for the Born collision term. Thus, a truncation of the Martin-Schwinger hierarchy at the second level and a neglect of higher-order terms lead to the Born collision term. In terms of Green's function diagrams, the result of Eq. (3.6) can be represented by the diagrams in Fig. 1.

As is well known, for the nuclear field, it is not possible to consider just the first few terms of the perturbation series for the corrections to the Green's functions, if one starts with the bare interaction $v_b(r_1,r_2)$. As a result, it is necessary to carry out partial summations so that some infinite sequence of terms of the perturbation series involving the bare interaction makes a first-order contribution involving the effective interaction to the quantities under consideration. The perturbation expansion (3.6) needs some amendment in order to be useful. For this purpose, we would like to examine in a formal way how the effective and the residual interactions are related to the bare interaction. It is convenient to introduce the vertex function for the bare interaction in the unantisymmetrized form:

$$\Gamma^{(0)}(12,34)=v_b(x_1,x_2)\delta(t_1-t_2)\delta(1-3)\delta(2-4)\,. \tag{3.7}$$

It is easy to show that the exact equation of motion involves the vertex function $\Gamma(12,34)$ in the form[36]

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\nabla_1{}^2\right)g(1,1')=\hbar\delta(1-1')+(-i)\int d2d3d4\Gamma(12,34)\mathcal{A}[g(3,1')g(4,2^+)]\,, \tag{3.8}$$

where the exact vertex function is given by the integral equation

$$\Gamma(12,34)=\Gamma^{(0)}(12,34)+\frac{i}{\hbar}\int d\bar{1}d\bar{2}d\bar{3}d\bar{4}\Gamma^{(0)}(12,\bar{3}\bar{4})g(\bar{3},\bar{1})g(\bar{4},\bar{2})\Gamma(\bar{1}\bar{2},34)\,. \tag{3.9}$$

[Equation (3.8), together with (3.9), is the same Eq. (10.15) of Ref. 36 except that in the last term of Eq. (3.8), we have used unantisymmetrized vertex functions but antisymmetrized Green's functions.] In general, the vertex function Eq. (3.9) cannot be solved exactly. One can, however, obtain an approximate solution, for example, by a partial sum involving compact diagrams to very high orders. Once this is accomplished, we identify the diagonal part of the vertex function as the effective interaction $v$ for the mean field:

$$\Gamma(12,34)=v(1,2)\delta(1-3)\delta(2-4)\text{ for }3=1\text{ and }4=2\,. \tag{3.10}$$

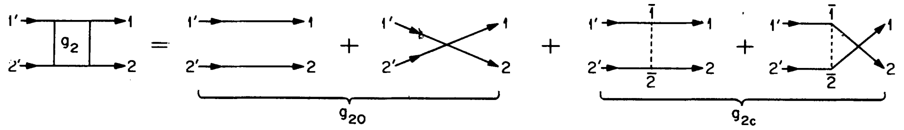


FIG. 1. Diagrammatic representation of the perturbation expansion of the two-body Green's function [Eqs. (2.10) and (3.6)], up to the first order in the interaction represented by a dashed line.

For the off-diagonal elements of the vertex function, as different space-time points are involved at the vertices, the simplest parametrization in terms of a residual interaction $v'$ can be given in the form

$$\Gamma(12,34)=v'(1,2)g(1,3)g(2,4)v'(3,4) \text{ for } 1\neq 3 \text{ and } 2\neq 4\,, \tag{3.11}$$

involving a second order in the interaction $v'$. This form is chosen as to correspond to the result of the perturbation expansion (3.6) involving, however, the residual interaction $v'$ instead of $v$. With these identifications, the equation of motion (3.8) becomes

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\nabla_1{}^2\right)g(1,1')=\hbar\delta(1-1')+(-i)\int d2v(1,2)\mathcal{A}[g(1,1')g(2,2^+)]+(-i)\int d2v'(1,2)g_{2c}(12,1'2^+)\,, \tag{3.12}$$

where

$$g_{2c}(12,1'2^+)=\frac{i}{\hbar}\int d\bar{1}d\bar{2}g(1,\bar{1})g(2,\bar{2})v'(\bar{1},\bar{2})\mathcal{A}[g(\bar{1},1')g(\bar{2},2^+)]\,. \tag{3.13}$$

We envisage that the mean-field theory of TDHF, obtained by using an effective interaction $v(1,2)$ in Eq. (3.12) and neglecting the residual interaction $v'(1,2)$ is a good approximate representation of the dynamics. In using an effective interaction having density dependence such as the Skyrme interaction and containing the effect of a rearrangement term because of such a dependence, many of the higher-order correlations are, in principle, included. It becomes now necessary to take into account the last term in Eq. (3.12) as a correction due to the residual interaction. In general, the effective interaction $v$ and the residual interaction $v'$ need not be the same.

Even though the perturbation expansion (3.13) we obtain for our Green's function is the same as that of Martin and Schwinger and Kadanoff and Baym, our Green's functions are defined with respect to nonequilibrium dynamical states in the real-time domain. The temporal path of integration needs to be carefully selected. Many investigations of the time-path for Green's function in the real-time domain have been carried out.[37-40] In particular, it can be shown that the perturbation expansion for the Green's function in the real-time domain for nonequilibrium (wave-packet-like) systems is identical with those of the zero-temperature perturbation theory; only the time-integration path and the path-ordering of the field operators are different. The path of time integration is such that times runs from $t_0$ before which the residual interaction vanishes to a time $t_\alpha$ after which the residual interaction is absent and then back from $t_\alpha$ to $t_0$ again. The ordering of the field operator in the evaluation of the expectation value is along the direction of the path; the further along the path, the "later" is the "time-path" in the ordering of the field operators. The justification for such a type of time path and path ordering has been discussed in detail and will not be repeated here.[37-40] Briefly, this type of time-integration path and path ordering arises because the Green's function is the expectation value of time-dependent field operators. Thus, in the evaluation of the expectation value, the time translation can be viewed as developing forward in time from the original state but later has to develop backward in time to reach the same original state. Some applications of this time-path method to obtain the kinetic equation, similar to the ones discussed here, have been presented previously.[38,39,40]

In our case, the residual interaction is present in the remote past and one can choose $t_0$ to be $-\infty$. For our purposes, it is sufficient to limit our attention to $t_1'=t_1$. The residual interaction is operative up to the present time $t_1$ under consideration, and thus one can choose $t_\alpha$ to be $t_1^-$, the negative superscript to indicate the limit $\lim_{\eta\to 0}(t_1-\eta)$ so as to avoid the singularity of the Green's functions at $t_1$. With this choice of time path and the path ordering for the Green's function in the real-time domain, the correlated part of the Green's function $g_{2c}$ of Eq. (3.13) is explicitly given for $t_1'=t_1^+$ by

$$\begin{aligned}g_{2c}(12,1'2^+)=\frac{i}{\hbar}\int d\bar{x}_1 d\bar{x}_2\int_{-\infty}^{t_1^-}d\bar{t}_1\{&g^>(1,\bar{1})g^>(2,\bar{2})v'(\bar{x}_1,\bar{x}_2)\mathcal{A}[g^<(\bar{1},1')g^<(\bar{2},2^+)]\\&-g^<(1,\bar{1})g^<(2,\bar{2})v(\bar{x}_1,\bar{x}_2)\mathcal{A}[g^>(\bar{1},1')g^>(\bar{2},2^+)]\}\,.\end{aligned} \tag{3.14}$$

This form of the correlated part of the two-body Green's function is also what is obtained by Kadanoff and Baym as one can deduce from their Eqs. (8-27a) and (8-29).[24,41] There, the result for Green's function in the real-time domain is obtained from those in the imaginary-time domain by analytic continuation.

With this result for the correlated part of the two-body Green's function, we obtain the following equation of motion for the one-body Green's functions for $t_1' = t_1^+$:

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2}{2m}\nabla_1{}^2 - U_{\mathrm{MHF}}(1)\right)g^<(1,1')$$
$$=\hbar\delta(1-1')+\frac{i}{\hbar}\int d2v'(1,2)d\bar{x}_1 d\bar{x}_2\int_{-\infty}^{t_1^-} d\bar{t}_1\{g^>(1,\bar{1})g^>(2,\bar{2})v'(\bar{x}_1,\bar{x}_2)\mathcal{A}[g^<(\bar{1},1')g^<(\bar{2},2^+)]$$
$$-g^<(1,\bar{1})g^<(2,\bar{2})v'(\bar{x}_1,\bar{x}_2)\mathcal{A}[g^>(\bar{1},1')g^>(\bar{2},2^+)]\}. \quad (3.15)$$

This is a closed equation involving only one-body Green's functions. It is the extension of the time-dependent Hartree-Fock approximation to include particle collisions. This equation can be called the extended TDHF approximation in Green's function form. The additional term [the last term of the above Eq. (3.15), or equivalently, the collision matrix $I(1,1')$ in Eq. (2.15)] is second order in the residual interaction, much as the collision term in the classical Boltzmann equation. Furthermore, because the integration over "past collision history" extends only from $\bar{t}_1 = -\infty$ to $\bar{t}_1 = t_1^-$, time reversal invariance is destroyed, much as in the Boltzmann equation. The only qualitative difference from the Boltzmann equation is its being non-Markovian in the sense that the equation for the Green's function depends not just on the Green's function at the time under consideration but also on the Green's function over the past collision history.

## IV. CHOICE OF TIME-DEPENDENT SINGLE-PARTICLE BASIS FUNCTIONS

Although the TDHF equation can be expressed either in the density matrix form or alternatively in the form of a set of single-particle equations (Appendix A), the practical application of TDHF is simpler when one deals with the single-particle equations rather than the density matrix.[9-12] Similarly, in the extended TDHF approximation the introduction of single-particle basis functions will simplify its practical application. A proper choice of the basis functions also allows a clean separation between the effects due to particle collisions and the effects due to the temporal variation of the mean field and thus makes the connection between the single-particle equations in the TDHF approximation and those in the ETDHF approximation very transparent.

The Green's function $g^<(x_1t_1, x_1't_1')$ is a matrix in $x_1t_1$ and $x_1't_1'$. We wish to represent it in terms of an orthonormal set of single-particle states $\psi_\lambda(xt)$. In general, this will lead to an occupation number matrix having diagonal and off-diagonal elements. The presence of the nondiagonal terms will lead to an equation for the number matrix with a sevenfold summation over the indices of the complete set of the basis single-particle states (Appendix B) and renders the dynamics rather intractable. To make the problem simple, we shall therefore specialize to an approximate representation of the Green's function in the form

$$-ig^<(x_1t_1, x_1't_1') = \sum_\lambda^\infty n_\lambda\left(\frac{t_1+t_1'}{2}\right)\psi_\lambda(x_1t_1)\psi_\lambda^*(x_1't_1'), \quad (4.1)$$

with the complementary Green's function

$$ig^>(x_1t_1, x_1't_1') = \sum_\lambda^\infty\left[1-n_\lambda\left(\frac{t_1+t_1'}{2}\right)\right]\psi_\lambda(x_1t_1)\psi_\lambda^*(x_1't_1'), \quad (4.2)$$

satisfying the identity

$$\lim_{t_1'\to t_1}[ig^>(x_1t_1, x_1't_1') - ig^<(x_1t_1, x_1't_1')] = \delta(x_1-x_1'). \quad (4.3)$$

The effect of particle collisions can be readily separated by choosing the complete set of single-particle states $\psi_\lambda$'s to satisfy the modified TDHF equation:

$$i\hbar\frac{\partial}{\partial t}\psi_\lambda(xt) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_{\mathrm{MHF}}(xt)\right)\psi_\lambda(xt), \quad (4.4)$$

where the potential $U_{\mathrm{MHF}}$ as defined by Eq. (2.14) is the same as the ordinary Hartree-Fock potential except that the occupation number is now time dependent. This choice of the single-particle state is a convenient one. For, upon constructing the equal-time Green's function and substituting into the equation of motion Eq. (2.15), many terms cancel out with the exception of $\partial n_\lambda/\partial t$ and $I(1,1')$. In fact, we have

$$\sum_{\lambda}^{\infty} \frac{\partial n_\lambda(t)}{\partial t} \psi_\lambda(x_1 t)\psi_\lambda^*(x_1' t^+) = -I(x_1 t, x_1' t^+)/\hbar\,. \tag{4.5}$$

Thus, the orthonormality of the basis function $\psi_\lambda(xt)$ leads to

$$\frac{\partial n_\lambda(t)}{\partial t} = -(1/\hbar)\int dx_1 dx_1' \psi_\lambda^*(x_1 t) \times I(x_1 t, x_1' t^+)\psi_\lambda(x_1' t)\,. \tag{4.6}$$

Thus, with the choice of basis states satisfying Eq. (4.4), the effect of collision is mainly to change the occupation probabilities of the single-particle states with time. Obviously, in the collisionless limit, our equation reduces to the TDHF equations with frozen occupation probabilities.

Equation (4.6) can, of course, be expressed completely in terms of the single-particle basis functions by means of Eqs. (3.15), (4.1), and (4.2). The resultant set of Eqs. (4.6) and (4.4) is closed in itself as it contains only the basis wave functions $\psi_\lambda(x,t)$ and the occupation probability $n_\lambda(t)$. However, this set of equations is non-Markovian as the time coordinate in the wave functions and the occupation numbers range from $-\infty$ to the present time $t_1^-$ and is therefore difficult to use directly. To be of good use, it is necessary to reduce the right-hand side of the Eq. (4.6) into a simple Markovian form. Our formulation will be complete when we succeed in such a reduction. The next section will be devoted to such a reduction for the special case of a slowly varying mean field.

As we remarked before, a more general representation of the one-body Green's function in terms of an occupation number matrix makes the dynamics rather intractable, although the equation of motion can be obtained in a similar way. For completeness, we present the results for the case with an occupation number matrix in Appendix B.

## V. SLOWLY VARYING MEAN-FIELD APPROXIMATION

The equation of motion (3.15) [or equivalently Eq. (4.6) in its unsimplified form], is non-Markovian and therefore cannot be of much use in practical calculations. It is desirable to reduce it into a Markovian form so that all the quantities in the equation of motion are specified at the same time coordinate. This requirement necessitates an integration over the collision history analytically. Obviously, this cannot be done in general but is possible in a special case where the mean field is varying slowly enough so that simplifying assumptions can be made concerning the temporal behavior of the Green's functions. As the assumptions are made only in connection with the evaluation of the collision term, which is only a correction term, refinement of these simplifying assumptions only leads to higher-order corrections and may therefore be less important.

Accordingly, in order to obtain $g_{2c}$ by integrating over past collision history, we shall consider the case in which the mean field is a slowly varying function of time. We substitute the representations (4.1) and (4.2) for the Green's function and perform the integration over $\bar{t}_1$. The Green's function is expected to peak sharply about the relative time coordinate[24] so that only a small region of $\bar{t}_1$ within a width of the correlation time is important in the integral of (3.14). We assume that the mean field varies so slowly that the typical time scale for the variation of the mean field is long compared with this correlation time. It is then reasonable to assume for the evaluation of $g_{2c}$ that the time dependence of the single-particle wave function satisfies the approximation

$$\psi_\lambda(x, T+\tfrac{1}{2}\tau) \simeq e^{-i\epsilon_\lambda(T)\tau/2\hbar}\psi_\lambda(xT)\,, \tag{5.1}$$

where $\epsilon_\lambda(T) = [\psi_\lambda(xT), h(T)\psi_\lambda(xT)]$ and $h(T)$ is the modified Hartree-Fock single-particle Hamiltonian defined by

$$h(t) = -\frac{\hbar^2}{2m}\nabla^2 + U_{\mathrm{MHF}}(x,t)\,. \tag{5.2}$$

Such an approximation is found to account quite well for the predominant time dependence of the TDHF single-particle wave functions for small time intervals of $\tau$.[42] Similarly, it is also reasonable to assume that

$$\epsilon_\lambda[(t_1+\bar{t}_1)/2] \simeq \epsilon_\lambda(t_1) \tag{5.3}$$

and

$$n_\lambda[(t_1+\bar{t}_1)/2] \simeq n_\lambda(t_1)\,. \tag{5.4}$$

From Eq. (3.14), the result of the integration over $\bar{t}_1$ gives the correlated part of the equal-time two-body Green's function:

$$g_{2c}(xt, x''t; x't^+, x''t^+) = \sum_{1234} [(1-n_1)(1-n_2)n_3 n_4 - n_1 n_2(1-n_3)(1-n_4)] \times (\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4-i\eta)^{-1}_{\eta\to 0}\,\psi_1(xt)\psi_2(x''t)\psi_3^*(x''t)\psi_4^*(x't)\,\langle 12|v'|43-34\rangle\,. \tag{5.5}$$

Thus, from Eq. (2.16), the equal-time collision matrix is given explicitly by

$$I(xt,x't^+) = -i\int dx''[v'(x,x'') - v'(x',x'')]$$
$$\times \sum_{1234} [(1-n_1)(1-n_2)n_3n_4 - n_1n_2(1-n_3)(1-n_4)]$$
$$\times (\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4-i\eta)^{-1}_{\eta\to 0}\,\psi_1(xt)\psi_2(x''t)\psi_3^*(x''t)\psi_4^*(x't)\,\langle 12|v'|43-34\rangle\,, \tag{5.6}$$

where the antisymmetrized matrix element $\langle 12|v'|43-34\rangle$ is given by

$$\langle 12|v'|43-34\rangle = \int dx\,dx'\,\psi_1^*(x)\psi_2^*(x')v'(x,x')[\psi_4(x)\psi_3(x') - \psi_3(x)\psi_4(x')]\,. \tag{5.7}$$

With this explicit form of the collision matrix, the scalar product with $\psi_1(x)$ and $\psi_1(x')$ can be readily obtained. From Eqs. (4.6) and (5.6), we find the master equation for the occupation probability:

$$\frac{\partial n_1(t)}{\partial t} = \frac{\pi}{\hbar}\sum_{234}\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)[(1-n_1)(1-n_2)n_3n_4 - n_1n_2(1-n_3)(1-n_4)]\,|\langle 12|v'|43-34\rangle|^2\,. \tag{5.8}$$

Together with Eq. (4.4), 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, the Pauli principle, and transition probabilities.[43] Thus, Eq. (5.8) can be used not only in ETDHF but also in other microscopic non-self-consistent descriptions of collective dynamics.

Our formulation of the extended TDHF made use of the Green's function and slowly varying mean field to arrive at the simple results of Eq. (4.4) and Eq. (5.8). An independent investigation using the Green's function formulation has also been undertaken by Shakin and Weiss.[6] They obtained equations similar to Eqs. (4.4) and (5.8) with the exception of the omission of the exchange term and the introduction of a correlation time $T$ resulting in the appearance of the function

$$\frac{\pi\sin|\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4|T}{|\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4|}$$

in the master equation which, with the proper addition of a small imaginary component to $\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4$, can be considered as a special representation of the $\delta$ function when $T$ approaches infinity.

As we shall see in the next section, a more refined form of the master equation can be obtained by taking the lifetime of the particle into account. In that case, the $\delta$ function in Eq. (4.4) needs to be replaced by a Lorentzian.[5] An independent investigation by Orland and Schaeffer[7] using also the Green's function formulation leads to similar results.

## VI. SUMMARY AND REFINEMENT OF ETDHF APPROXIMATION

In the previous sections, we have shown how the ETDHF approximation can be written in the non-Markovian form and how in the case of slowly varying mean field the results can be reduced to the Markovian form so that the explicit history is not used to describe the present state. For practical applications, obviously, it is desirable to work with the ETDHF approximation in the latter form. We shall henceforth focus our attention on such a formulation, keeping in mind the limitations with regard to the slow variation of the mean field.

We hereby summarize the main results of the ETDHF approximation (in the Markovian form). We select a complete set of time-dependent basis states $\psi_\lambda(x,t)$ to separate the effects due to the mean field and the effects due to particle collisions. The complete set $\psi_\lambda(x,t)$ is chosen to satisfy the modified time-dependent Hartree-Fock equation

$$i\hbar\frac{\partial}{\partial t}\psi_\lambda(xt) = \left(-\frac{\hbar^2}{2m}\nabla^2 + U_{\rm MHF}(xt)\right)\psi_\lambda(xt)\,, \tag{6.1}$$

such that the effect of collision can be included in terms of a variation of a time-dependent occupation number $n_\lambda(t)$ for the single-particle state $\psi_\lambda(xt)$ where $\lambda$ runs from 1 to infinity. The modified Hartree-Fock potential is defined as

$$U_{\rm MHF}(xt)\psi_\lambda(xt) = \int dx_2\,\rho(x_2)v(x,x_2)\psi_\lambda(xt) - \int dx_2\sum_{\lambda'} n_{\lambda'}\psi_{\lambda'}(x)\psi_{\lambda'}^*(x_2)v(x,x_2)\psi_\lambda(x_2)\,. \tag{6.2}$$

The interaction $v(x,x_2)$ can be density dependent in which case it must include the rearrangement terms.

The density $\rho(x)$ is given by

$$\rho(x)=\sum_{\lambda} n_{\lambda}(t)\psi_{\lambda}(xt)\psi_{\lambda}^{*}(xt)\,. \tag{6.3}$$

The occupation numbers $n_{\lambda}$ for the single-particle states now satisfy the master equation:

$$\frac{\partial n_1}{\partial t}=\frac{\pi}{\hbar}\sum_{2,3,4}\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)[(1-n_1)(1-n_2)n_3n_4-n_1n_2(1-n_3)(1-n_4)]\,|\langle 12|v'|43-34\rangle|^2\,, \tag{6.4}$$

where we have used the abbreviated subscripts 1, 2, 3, and 4 to stand for the state labels $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$, respectively. The matrix element of the residual interaction $v'$ is defined as

$$\langle 12|v'|43-34\rangle=\int dx dx'\psi_1^{*}(x)\psi_2^{*}(x')v'(x,x')[\psi_4(x)\psi_3(x')-\psi_3(x)\psi_4(x')]\,, \tag{6.5}$$

and the single-particle energies $\epsilon_{\lambda}$ are

$$\epsilon_{\lambda}(t)=\int dx\psi_{\lambda}^{*}(xt)\left(-\frac{\hbar^2}{2m}\nabla^2+U_{\mathrm{MHF}}(xt)\right)\psi_{\lambda}(xt)\,. \tag{6.6}$$

It is easy to cast Eq. (6.4) in terms of transition probabilities by taking note of Fermi's "golden rule" that the transition probability $W(12;34)$ is related to the matrix element by

$$W(12;34)=(2\pi/\hbar)\,|\langle 12|v'|43-34\rangle|^2\,, \tag{6.7}$$

which leads to

$$\frac{\partial n_{\lambda}}{\partial t}=\frac{1}{2}\sum_{234}W(12;34)\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)[n_3n_4(1-n_1)(1-n_2)-n_1n_2(1-n_3)(1-n_4)]\,. \tag{6.8}$$

We note in passing that in Eq. (6.8) the summation over the final states 3 and 4 is unrestricted so that a given pair of final states appear twice in the summation (state $3=\alpha$, state $4=\beta$, and state $3=\beta$, state $4=\alpha$). One can introduce a restricted summation $\sum_{2,\{3,4\}}$ such that each combination of final states 3 and 4 appear only once. In the form of the restricted summation, Eq. (6.8) becomes

$$\frac{dn_{\lambda}}{dt}=\sum_{2\{3,4\}}W(12;34)\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)[n_3n_4(1-n_1)(1-n_2)-n_1n_2(1-n_3)(1-n_4)]\,, \tag{6.9}$$

which is identical to the usual form of the master equation in the literature [see, e.g., Eq. (1.147) of Ref. 43].

Our approximate result (6.4) makes use of only the expectation values of the single-particle Hamiltonian and occupation numbers whose time dependence is slow enough that Eqs. (5.3) and (5.4) are good approximations. However, one finds from the subsequent result of the master Eq. (6.4) that a particle in a single-particle state has a finite lifetime (Sec. IX). To the lowest order of approximation, the occupation probability varies in time according to the exponential decay law:

$$n_{\lambda}\left(\frac{t_1+\bar{t}_1}{2}\right)\simeq n_{\lambda}(t_1)\exp[-\Gamma_{\lambda}(\bar{t}_1-t_1)/2\hbar]\,, \tag{6.10}$$

where the width $\Gamma_{\lambda}$ is related to the inverse of the lifetime of this particle in the single-particle state $\lambda$

$$\Gamma_{\lambda}=\hbar/\tau_{\lambda}\,. \tag{6.11}$$

The master equation can therefore be refined in a self-consistent manner in which the derivation of the collision matrix takes into account this temporal dependence of the occupation number. Operationally, in the evaluation of the collision matrix, this dependence of $n_{\lambda}$ on $(\bar{t}_1-t_1)$ is equivalent to an occupation number having no such dependence but with the single-particle energy $\epsilon_i$ replaced by $\epsilon_{\lambda}-i\Gamma_{\lambda}/2$. When this is taken into account the master equation appears in the same form as that of Eq. (6.4), except that now the $\delta$ function in energies is replaced by a Lorentzian

$$\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)\to D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)=\frac{1}{2\pi}\,\frac{\Gamma_{1234}}{(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)^2+(\Gamma_{1234}/2)^2}\,, \tag{6.12}$$

where

$$\Gamma_{1234}=\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4\,. \tag{6.13}$$

A self-consistent treatment of the width for all the single-particle states is probably a rather formidable undertaking. A simpler treatment is to assume that since the most important effects of the collision process occur with nucleons in the velocity of the Fermi surface, it is possible to introduce an average width Γ for all the single-particle states resulting in a width parameter in the distribution $D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ in (6.12) independent of the states. The implementation of the ETDHF can then be greatly simplified. Other types of distribution can also be useful. For example, instead of the distribution (6.12), one can follow Shakin and Weiss to introduce a correlation time $T$ to represent the distribution[6] as

$$D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)=\frac{\pi\sin|\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4|\,T}{|\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4|} \tag{6.14}$$

or as a distribution as those used in Strutinsky's shell correction method[44]:

$$D(x)=\frac{1}{\sqrt{\pi}}\,e^{-(x^2/4\Gamma^2)}\sum_{k=0}^{m} a_{2k}H_{2k}(x/2\Gamma)\,, \tag{6.15}$$

where $x=\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4$,

$$a_{2k}=-(1/4k)a_{2k-2} \text{ for } k>0 \text{ with } a_0=1\,,$$

and $H_{2k}$ is the Hermite polynomial of order $2k$. The advantage of distributions of the type (6.14) and (6.15) is that as they assume negative, as well as positive, values, they may lead to better convergence in a numerical calculation. Clearly, much experimentation is needed to find the best distribution function for future numerical implementation of the ETDHF approximation. However, because of their not always being positive definite, the $H$ theorem concerning the non-negative nature of the rate of change of entropy cannot be obtained (Sec. VIII).

It is easy to see that in the absence of residual interactions, our set of equations reduces to the usual TDHF equation as a collisionless limit with frozen occupation probabilities.

With regard to the total particle number, we note that upon taking the summation of Eq. (6.4) with respect to the state label λ, we obtain

$$\frac{\partial}{\partial t}\sum_{\lambda} n_\lambda=0\,, \tag{6.16}$$

which remains true even when the δ function is replaced by a distribution $D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ symmetrical with respect to the interchange of $\epsilon_1\rightleftarrows\epsilon_4$ and $\epsilon_2\rightleftarrows\epsilon_3$ such as Eqs. (6.12), (6.14), and (6.15). Thus, in our set of equations of motion, the total number of particles is rigorously conserved. There is no need here to introduce a Lagrange multiplier to conserve a particle number as was done previously by Shakin and Weiss.[6]

So far, the results obtained are general and include the spatial, spin, and isospin degrees of freedom. However, for some practical problems, it is often desirable to restrict ones attention to only the spatial degree of freedom, while the spin and isospin degrees of freedom are averaged over. We shall show in Appendix C how this is done in the case when the residual interaction depends only on the spatial coordinates.

## VII. SIMPLE ANALYTIC SOLUTIONS OF THE MASTER EQUATION FOR FOUR ISOLATED STATES

The set of occupation number equations are coupled to the modified Hartree-Fock equation through the two-body matrix element. They run through the whole set of occupation numbers of all the single-particle states. In order to obtain some clear insight into the physics involved, we shall consider the special case of four isolated states and look for the analytic solutions of the master Eq. (6.4). Here, we have a coupled set of equations for $\partial n_i/\partial t$, where $i=1,2,3,4$. Because of the symmetry which exists in the factor containing the occupation numbers in the master equation, it is convenient to work with generalized occupation numbers $S$(sum), $F$, $D_1$(difference), and $D_2$(difference) related to the occupation numbers $n_i$ by the linear transformation:

$$S=n_1+n_2+n_3+n_4\,, \tag{7.1}$$

$$F=n_1+n_2-n_3-n_4\,, \tag{7.2}$$

$$D_1=n_1-n_2\,, \tag{7.3}$$

and

$$D_2=n_3-n_4\,. \tag{7.4}$$

One finds that

$$\frac{\partial S}{\partial t}=\frac{\partial D_1}{\partial t}=\frac{\partial D_2}{\partial t}=0\,, \tag{7.5}$$

which leads to the useful result that $S$, $D_1$, and $D_2$ are constants independent of time. The only equation that we need to solve is

$$\frac{\partial F(t)}{\partial t}=\frac{-\pi}{2\hbar}\,|\langle 12|v'|43-34\rangle|^2 \times\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)w(F,S,D_1,D_2)\,, \tag{7.6}$$

where the function $w$ is a polynomial cubic in $F$ given by

$$w(F,S,D_1,D_2)=F\,[F^2+4S(1-S/4)-2(D_1^2+D_2^2)] -4(1-S/2)(D_1^2-D_2^2)\,. \tag{7.7}$$

For simplicity of notation, we shall introduce the constant $a$ (which may be complex) and the real constant $b$ to write the above polynomial $w$ in the form

$$w(F) = F(F^2 + a^2) + b\ , \tag{7.8}$$

where

$$a^2 = 4S(1 - S/4) - 2(D_1^2 + D_2^2)\ , \tag{7.9}$$

and

$$b = -4(1 - S/2)(D_1^2 - D_2^2)\ . \tag{7.10}$$

To turn the relation given by (7.6) into a proper equation of motion for $F$, we make the assumption that the "levels" $E_A = \epsilon_1 + \epsilon_2$ and $E_B = \epsilon_3 + \epsilon_4$ are linear functions of time and cross at $t = t_0$. We assume further that the absolute square of the residual interaction matrix element varies slowly enough so that it can be taken to be a constant. Then, we obtain the equation of motion for $F$ as

$$\frac{dF(t)}{dt} = -\frac{\pi}{4} G^2[F(F^2 + a^2) + b]\delta(t - t_0)\ , \tag{7.11}$$

where we have converted the $\delta$ function of energy into that of time, and we have introduced $G^2$ as

$$G^2 = \frac{2}{\hbar} |\langle 12|v'|43 - 34\rangle|^2 \bigg/ \left|\frac{d(E_A - E_B)}{dt}\right|\ . \tag{7.12}$$

With $G^2$ independent of time and $w$ a cubic polynomial of $F$, the equation (7.11) can be solved analytically. We shall discuss the types of solutions for level crossings of three different kinds characterized by the different (but constant) values of $D_1$ and $D_2$. We name a level crossing to be of the first kind when the differences $D_1$ and $D_2$ are zero. This is the case when $n_1 - n_2 = n_3 - n_4 = 0$. The solution for this case is particularly simple. We name a level crossing to be of the second kind either (i) when the differences obey $D_1 = \pm D_2 \neq 0$, or (ii) when the total occupation number $S = 2$. We name a level crossing to belong to that of the third kind when the initial occupation numbers are arbitrary. This is the most general case for a system of four isolated states and the solution is slightly more complicated. We shall discuss these three kinds of level crossing separately.

### A. Level crossing of the first kind

The level crossing of the first kind is the special case in which initially, $n_1 = n_2$ and $n_3 = n_4$. We see from the constancy of $D_1 = (n_1 - n_2)$ that $n_1$ remains to be equal to $n_2$ if they are initially equal. Similarly, $n_3$ remains to be equal to $n_4$ if they are initially equal. In this case, Eq. (7.11) is greatly simplified to become

$$\frac{\partial F(t)}{\partial t} = -\frac{\pi}{4} G^2 F(F^2 + a^2)\delta(t - t_0)\ , \tag{7.13}$$

where $a^2$, as given by (7.9), assumes the special value

$$a^2 = 4S(1 - S/4)\ , \tag{7.14}$$

and $a^2 \geqslant 0$. The solution to Eq. (7.13) is readily obtained by direct integration. It is given by

$$\begin{aligned} n_1(t) &= n_2(t) \\ &= \tfrac{1}{2}[(n_{10} + n_{30}) + (n_{10} - n_{30}) f(t)] \end{aligned} \tag{7.15}$$

and

$$\begin{aligned} n_3(t) &= n_4(t) \\ &= \tfrac{1}{2}[(n_{10} + n_{30}) - (n_{10} - n_{30}) f(t)]\ , \end{aligned} \tag{7.16}$$

where $n_{i0}$ are the initial values of $n_i$ before the levels $E_A$ and $E_B$ cross. The time dependence is governed by the function $f(t)$ given by

$$f(t) = \left\{\left[1 + \left(\frac{F_0}{a}\right)^2\right] e^{(\pi/2)a^2 G^2 \theta(t - t_0)} - \left(\frac{F_0}{a}\right)^2\right\}^{-1/2}\ , \tag{7.17}$$

where

$$F_0 = n_{10} + n_{20} - n_{30} - n_{40}\ , \tag{7.18}$$

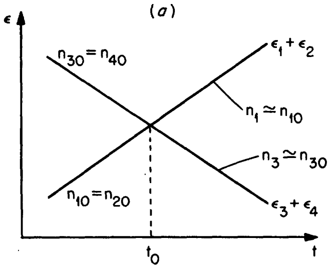
and $\theta$ is the usual step function.

Solutions of the level crossing of the first kind given by Eqs. (7.15)–(7.18) represent a physically simple but interesting situation. The jump discontinuity of the step function leads to redistributions of occupation numbers after the levels cross at $t = t_0$. This kind of level crossing has the following distinct features. If the rate of change of the energy difference, $|d(E_A - E_B)/dt|$, is large, or if the matrix element of $v'$ is small, then $G^2$ is small. Accordingly, the occupation numbers are essentially unchanged for $t > t_0$. This situation is depicted by Fig. 2(a). On the other hand, if the reverse is true, that is, if $|d(E_A - E_B)/dt|$ is small, or if the matrix element of $v'$ is large, then $G^2$ will be large; the solution (7.15)–(7.18) gives $n_1 \sim n_3 \sim \frac{1}{2}(n_{10} + n_{30})$, as illustrated schematically by Fig. 3(b). Such a redistribution can be easily understood. For, in this case of large $G^2$, the master equation becomes at $t = t_0^+$,

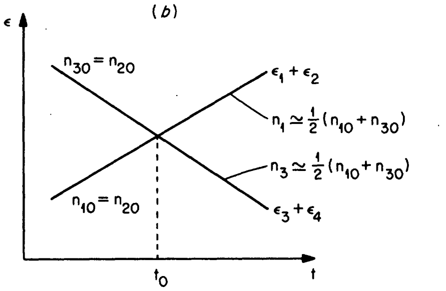
$$n_1 n_2(1 - n_3)(1 - n_4) - n_3 n_4(1 - n_2)(1 - n_3) \to 0\ , \tag{7.19}$$

which admits $n_1 = n_2 = n_3 = n_4$ as the solution when there are the initial constraints $n_1 = n_2$ and $n_3 = n_4$.

It is of interest to compare and contrast our results with the Landau-Zener level-crossing formula. There, one can consider also two-particle states $E_A$ and $E_B$ and a residual interaction such that $G^2$ of Eq. (7.12) is the same as the parameter $G^2$ which appears in the Landau-Zener formula



$G^2$ SMALL (RAPID MOTION OR SMALL INTERACTION)



$G^2$ LARGE (SLOW MOTION OR LARGE INTERACTION)

FIG. 2. The redistribution of the occupation probabilities in level crossings of the first kind where the occupation probability $n_1$ is equal to $n_2$ and $n_3$ is equal to $n_4$. The occupation probabilities are unchanged when $G^2$ is small, which is the case when the motion is rapid or when the interaction matrix element is small (a). The occupation probabilities are evenly divided among the four single-particle states when $G^2$ is large, which is the case when the motion is slow or when the interaction matrix element is large (b).

(e.g., Fig. 34 of Ref. 45). Our result is the same as that of Landau-Zener for small values of $G^2$, as they should be. However, for large values of $G^2$ (when either the collective motion is slow or when the matrix element is large), only the lowest level is occupied in a Landau-Zener level crossing in contradistinction to our case where the occupation probabilities are evenly distributed between the upper and the lower levels after the levels cross. Such a difference arises from the special ways of including correlations in our problem. Specifically, to arrive at our Markovian form of equation of motion, we evaluate, in essence, the two-body correlation anew at every instant of time by propagating backward in time, allowing a collision to take place and then propagating forward in time. Once such a correlation is obtained, at the present time, say, the past collision history is "erased" and the correlation in the future time has to be reworked again. In contrast, in the Landau-Zener case, all the correlations from the past to the present and to the future are kept intact. There is no such "erasing" of memory so that a coherent propagation of correlation is maintained. It is clear that for a system with only a few particles for which the coherent phase information can be kept throughout, the Landau-Zener formula is more suitable. However, for a system with a large number of particles, statistical treatment of the present kind will be simpler and more appropriate. In fact, one can easily see that irrespective of the initial distribution of the occupation numbers, it is our kind of redistribution which eventually gives rise to a Fermi-Dirac distribution characterized by a temperature.

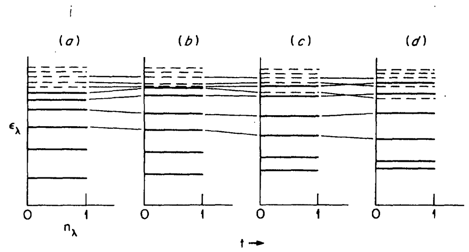


FIG. 3. Scenario for a nonequilibrium system which has not achieved thermal equilibrium. The solid line indicates occupied levels and the dashed line the unoccupied levels. The movement of the single-particle states is indicated by the thin lines between the subplots. The unequilibrated system evolves from (a) to (d) as time proceeds.

### B. Level crossing of the second kind

The simplifications of the solution in the previous subsection can be ultimately traced back to the fact that in the polynomial $w$ given in (7.8), we have specialized to the case where

$$b=-4(1-S/2)(D_1^2-D_2^2)=0\,. \tag{7.20}$$

For a level crossing of the second kind, we have either (i) $n_1-n_2=\pm(n_3-n_4)\neq 0$, or (ii) $S=2$. The same equality (7.20) again holds. Thus, Eq. (7.11) leads to the same time-dependent function $f(t)$. When the initial values of the occupation numbers are taken into account, one obtains the general solution for a level crossing of the second kind:

$$n_1(t)=\tfrac{1}{4}[(3n_{10}-n_{20}+n_{30}+n_{40}) + (n_{10}+n_{20}-n_{30}-n_{40})f(t)]\,, \tag{7.21}$$

$$n_2(t)=\tfrac{1}{4}[(-n_{10}+3n_{20}+n_{30}+n_{40}) + (n_{10}+n_{20}-n_{30}-n_{40})f(t)]\,, \tag{7.22}$$

$$n_3(t)=\tfrac{1}{4}[(n_{10}+n_{20}+3n_{30}-n_{40}) -(n_{10}+n_{20}-n_{30}-n_{40})f(t)]\,, \tag{7.23}$$

and

$$n_4(t)=\tfrac{1}{4}[(n_{10}+n_{20}-n_{30}+3n_{40}) -(n_{10}+n_{20}-n_{30}-n_{40})f(t)]\,, \tag{7.24}$$

where $f(t)$ is given by (7.17) except that the constant $a^2$ is now given by the general expression of Eq. (7.9) instead of the special value of Eq. (7.14).

Similar to the previous case, in the limiting case of very small $G^2$, the occupation numbers remain practically unchanged after level crossing. In the other extreme of large $G^2$, however, they are redistributed accordingly in the following approximate way:

$$n_1 \sim \tfrac{1}{4}(n_{10}+n_{20}+n_{30}+n_{40}) + \tfrac{1}{2}(n_{10}-n_{20}) , \tag{7.25}$$

$$n_2 \sim \tfrac{1}{4}(n_{10}+n_{20}+n_{30}+n_{40}) - \tfrac{1}{2}(n_{10}-n_{20}) , \tag{7.26}$$

$$n_3 \sim \tfrac{1}{4}(n_{10}+n_{20}+n_{30}+n_{40}) + \tfrac{1}{2}(n_{30}-n_{40}) , \tag{7.27}$$

and

$$n_4 \sim \tfrac{1}{4}(n_{10}+n_{20}+n_{30}+n_{40}) - \tfrac{1}{2}(n_{30}-n_{40}) . \tag{7.28}$$

Thus, when the collective motion is slow or when the interaction matrix element is large, the occupation numbers are redistributed in such a way that the sum and difference of $n_1$ and $n_2$ become equal to the corresponding sum and difference of $n_3$ and $n_4$.

### C. Level crossing of the third kind

The level crossing of the third kind is the general case for which the initial values of $n_1$, $n_2$, $n_3$, and $n_4$ are completely arbitrary. Even in this case, it is remarkable that Eq. (7.11) admits an analytic solution in a simple form which contains the solutions of the previous cases. To obtain this general solution, one notes that the polynomial $w$ can be rewritten in the factorized form:

$$w(x) = (x-\gamma)[x^2+\gamma x+(a^2+\gamma^2)] , \tag{7.29}$$

where $\gamma$, without loss of generality, is a real root of $w(x)=0$ and satisfies the equation

$$w(\gamma) = \gamma(\gamma^2+a^2)+b=0 . \tag{7.30}$$

Applying the method of partial fractions one arrives at the following solution after some tedious, but simple, algebraic manipulations:

$$n_1(t) = \bar{n} + \tfrac{1}{2}D_1 + \tfrac{1}{4}F_0\alpha(t) - \tfrac{1}{4}\gamma\beta(t) , \tag{7.31}$$

$$n_2(t) = \bar{n} - \tfrac{1}{2}D_1 + \tfrac{1}{4}F_0\alpha(t) - \tfrac{1}{4}\gamma\beta(t) , \tag{7.32}$$

$$n_3(t) = \bar{n} + \tfrac{1}{2}D_2 - \tfrac{1}{4}F_0\alpha(t) + \tfrac{1}{4}\gamma\beta(t) , \tag{7.33}$$

and

$$n_4(t) = \bar{n} - \tfrac{1}{2}D_2 - \tfrac{1}{4}F_0\alpha(t) + \tfrac{1}{4}\gamma\beta(t) , \tag{7.34}$$

where

$$\bar{n} = \tfrac{1}{4}(n_{10}+n_{20}+n_{30}+n_{40}) , \tag{7.35}$$

$$\alpha(t) = \left\{ f^2\left[1+\frac{3\gamma^2}{a^2}\left(4+3\left(\frac{F_0-\gamma}{a}\right)^2 f^2\right)\right]\right\}^{1/2} , \tag{7.36}$$

and

$$\beta(t) = \alpha(t) + \frac{3}{2}\left(\frac{F_0-\gamma}{a}\right)^2 f^2(t) - 1 , \tag{7.37}$$

with

$$F_0 = n_{10}+n_{20}-n_{30}-n_{40} ,$$

$$f(t) = \left\{\left[1+\left(\frac{F_0-\gamma}{a}\right)^2 - \frac{3\gamma F_0}{a^2}\right]\exp\left[\tfrac{1}{2}\pi G^2(a^2+3\gamma^2)\theta(t-t_0)+\gamma(\eta(F)-\eta(F_0))\right] - \left(\frac{F_0-\gamma}{a}\right)^2\right\}^{-1/2} , \tag{7.38}$$

and

$$\eta(x) = \frac{3}{(4a^2+3\gamma^2)^{1/2}} \tan^{-1}\frac{(4a^2+3\gamma^2)^{1/2}}{2x+\gamma} . \tag{7.39}$$

Thus, the functions $\alpha(t)$ and $\beta(t)$ appearing in the solutions (7.31)–(7.34) can be written analytically in terms of the function $f(t)$. The latter quantity, however, contains a function of the unknown

$$F(t) = n_1(t)+n_2(t)-n_3(t)-n_4(t) . \tag{7.2}$$

The final result needs to be obtained in an iterative manner when one uses (7.31)–(7.39).

As a limiting case, when $\gamma=0$ (i.e., when $b=0$), $f$ is simplified to the same expression as given by Eq. (7.14) and $\alpha=f$, thus recovering the solutions (7.15)–(7.16), and (7.21)–(7.24) for the level crossing of the first and second kind.

The step function $\theta(t-t_0)$ in all these solutions [Eqs. (7.17) and (7.38)] results from the integration of the $\delta$ function in time. When we allow for the finite lifetime of the single-particle states, the energies $\epsilon_i$'s will then take complex values and the $\delta$ function is replaced by the Lorentzian given in (6.12). The solutions given by (7.17) and (7.38) are then only modified by the following replacement:

$$\theta(t-t_0) \to \frac{1}{\pi}\tan^{-1}\left(2\left|\frac{d(E_A-E_B)}{dt}\right|(t-t_0)/\Gamma_{1234}\right)+\frac{1}{2} . \tag{7.40}$$

where $\Gamma_{1234}$ has been defined in (6.13).

## VIII. THE ENTROPY, *H* THEOREM, AND THERMAL EQUILIBRIUM

The coupled equations (6.1) and (6.4) we obtained are just the configuration-space analog of the quantum Boltzmann equation. It is applicable to both finite and infinite systems. For an infinite system, the energy levels are no longer discrete and the states can be labeled by the momentum state $k$. The master equation for the occupation number becomes the usual Uehling and Uhlenbeck equation[30] for an infinite system. As with the quantum Boltzmann equation of Uehling and Uhlenbeck from which much information concerning conservation laws and the approach to equilibrium can be obtained, so it is with the coupled equations (6.1) and (6.4) presented here for our systems. We shall begin first by proving the well-known *H* theorem that entropy never decreases.

We introduce the entropy density to be

$$\sigma(x,t) = -k_B \sum_{\lambda} \psi_\lambda(xt)\psi_\lambda^*(xt)\,\{n_\lambda(t)\ln n_\lambda(t) + [1-n_\lambda(t)]\ln[1-n_\lambda(t)]\}\,, \tag{8.1}$$

where $k_B$ is the Boltzmann constant. Accordingly, the total entropy of the system is given as

$$S(t) = \int dx\,\sigma(x,t) = -k_B \sum_{\lambda} \{n_\lambda(t)\ln n_\lambda(t) + [1-n_\lambda(t)]\ln[1-n_\lambda(t)]\}\,. \tag{8.2}$$

We now consider the time rate of change of entropy

$$\frac{dS(t)}{dt} = \frac{-\pi k_B}{\hbar} \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \delta(\epsilon_{\lambda_1}+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4})\,|\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle|^2$$
$$\times[(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4} - n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_1})(1-n_{\lambda_4})]\ln\left(\frac{n_{\lambda_1}}{1-n_{\lambda_1}}\right), \tag{8.3}$$

where we have applied the master equation (6.4) to eliminate $\dot{n}_\lambda$. Exchanges of the indices $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$ among themselves lead to different representations of the same expression. This gives

$$\frac{dS(t)}{dt} = \frac{-\pi k_B}{4\hbar} \sum_{\lambda_1\lambda_2\lambda_3\lambda_4} \delta(\epsilon_{\lambda_1}+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4})|\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle|^2$$
$$\times[(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4} - n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})]\ln\left(\frac{n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})}{(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4}}\right). \tag{8.4}$$

For any combination of $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$, the product of the factor containing $n_\lambda$'s and the logarithmic term is of the form $(x-y)\ln(y/x)$, which is easily shown to be negative definite. Hence, we have arrived at the *H* theorem which states that

$$dS(t)dt \geq 0\,. \tag{8.5}$$

It is easy to see further from (8.4) that the equality of the above expression occurs if and only if for any $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$, we have

$$[(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4} - n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})]\ln\left(\frac{n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})}{(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4}}\right) = 0\,, \tag{8.6}$$

which is equivalent to the condition that for any $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$,

$$(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4} - n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4}) = 0\,, \tag{8.7}$$

leading to $\partial n_\lambda/\partial t = 0$. Thus, when the entropy of the system becomes stationary, so do the occupation numbers.

It is clear from the arguments given above that the conclusion reached in Eqs. (8.5) and (8.7) remains valid when the $\delta$ functions in the master equation are replaced by the Lorentzian distribution function $D(\epsilon_{\lambda_1}+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4})$ of Eq. (6.12) [but not by distribution functions of Eqs. (6.14) and (6.15)].

With the *H* theorem, we have a way to measure how far a nonequilibrium system is from thermal equilibrium by calculating the rate of change of the entropy. The analytic solutions we have developed in the last section also help us understand in a microscopic way how a nonequilibrium system approaches equilibrium.

The collision process we are considering is a real process and is therefore subject to the restriction of energy conservation. This restriction on the exact equality of $\epsilon_{\lambda_1}+\epsilon_{\lambda_2}$ and $\epsilon_{\lambda_3}+\epsilon_{\lambda_4}$ may be relaxed slightly when one considers the possibility of a width for the single-particle states. How is such a near equality achieved in order to have the occurrence of a "collision"? It is achieved by the dynamical motion of the system, thereby a change in the mean field and the kinetic energy of the particles bring about a change in the values of $\epsilon_\lambda$. The change of $\epsilon_\lambda$ as a function of time then gives rise to accidental near equality of the levels $E_A$ and $E_B$, an occurrence which we call level crossing, and a "collision" then takes place to rearrange the occupation probabilities of the four different single-particle states. It is in this context that level crossings, particularly from those involving states near the Fermi surface, are very important in the discussion of the approach to thermal equilibrium.

It is instructive to devise a scenario for the occurrence or nonoccurrence of thermalization, based on the analytic results we have obtained. For simplicity of discussion, we shall consider level crossings of the first kind and take states $\lambda_1$ and $\lambda_2$ (and similarly $\lambda_3$ and $\lambda_4$) to belong to the same single-particle level and the same time-reversal doublet. In this case, levels $E_A$ and $E_B$ will cross when the single-particle states $\epsilon_{\lambda_1}$ and $\epsilon_{\lambda_3}$ have a level crossing. The matrix element appearing in Eq. (7.12) has the magnitude of the pairing mixing element. This matrix element is so much greater than the average matrix elements of the other types that we can neglect level crossings of the third kind for our qualitative description of the thermalization process. Level crossings of the second kind have qualitative features much like those of the first kind and need not be discussed separately.

We have now the following scenario for a system which does not achieve thermal equilibrium. We can envisage that at time $t=0$ the single-particle levels $\epsilon_\lambda$ of a system are arranged as in Fig. 3(a) with the occupation number indicated by the lengths of the solid lines. As the time proceeds, the change of the mean field, as well as the dynamics, will result in a shift in the positions of the levels. Such a shift is indicated in Fig. 3 by lines joining the levels for a few of those levels near the Fermi surface. For example, there can be a level crossing on top of the Fermi sea, as illustrated in Fig. 3(b). We can envisage a situation in which the dynamics proceeds in such a rapid manner that the parameter $G^2$ in Eq. (7.12) is very small so that after level crossing (of the first kind) takes place, the occupation number remains unchanged. The system will reach the configuration at Fig. 3(d) at a later time. As unoccupied states now lie below occupied states, this is not a thermalized system.

Thermalization takes place when the dynamical motion is sufficiently slow. We have the following scenario for a system in a slow motion depicted in Fig. 4. Now, when a level crossing on top of the Fermi sea takes place in Fig. 4(b), a redistribution of the occupation probabilities takes place to divide them evenly between the two levels [Fig. 4(c)]. If further level crossings take place as in Fig. 4(d), the occupation probabilities are further redistributed to give a smooth tail for the occupation probabilities. It is this kind of redistribution which leads eventually to a Fermi-Dirac distribution of occupation probabilities characterized by a finite temperature.

So far, the thermalization process is discussed with regard to the influence of the speeds of the dynamics. There is another important factor which also enters into the process of thermalization. Clearly, the larger the number of levels which cross at the top of the Fermi sea, the greater will be the rearrangement of the occupation probabilities. The thermalization process proceeds more readily when the density of single-particle states at the Fermi surface is high.

It is possible to put all the above discussions in slightly more quantitative terms by finding from the master equation (6.4) a time scale with respect to which the dynamics is considered slow or fast. For systems not far from equilibrium, $\partial n_\lambda/\partial t \sim 0$ for states $\lambda$ much above or much below the Fermi surface. We focus our attention on the occupation number for states $\lambda$ near the Fermi surface for which the factor containing the occupa-

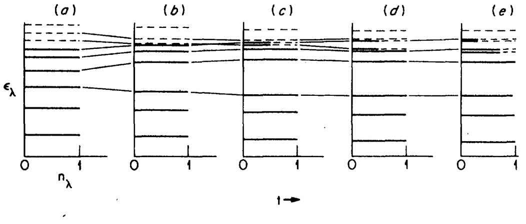


FIG. 4. Scenario for a nonequilibrium system to approach thermal equilibrium. The length of the solid line indicates the degree of occupancy of the single-particle states, while the length of the thin dashed line the degree of emptiness. The movement of the single-particle states are indicated by thin lines. As time proceeds, the system evolves from (a) and (b), then (c), then (d), and then (e). In (b) and (d), we show the occurrence of level crossing, with the resultant redistribution of occupation probabilities shown in the subsequent subplot.

tion numbers in the square bracketed expression of E. (6.4) assumes a value of the order of $\frac{1}{2}$. We restrict ourselves to the case where $\lambda_1$ and $\lambda_2$ (and also $\lambda_3$ and $\lambda_4$) are time-reversal doublets. We can give a value of 2 MeV as the average value of the matrix element[46] and obtain

$$\frac{\partial n_\lambda}{\partial t} \sim \frac{\rho(\epsilon_f)}{2} \times \frac{\pi}{\hbar} (2 \text{ MeV})^2 \times \frac{1}{2}, \tag{8.8}$$

where $\rho(\epsilon_f)$ is the density of single-particle states at the Fermi surface and is given on the average by[44]

$$\rho(\epsilon_f) \sim \tfrac{3}{40} A \text{ MeV}^{-1}. \tag{8.9}$$

Thus, we have the approximate rate of change of the occupation probability

$$\frac{\partial n_\lambda}{\partial t} \sim 1.2 \times 10^{-3} A \ (\text{fm}/c)^{-1}. \tag{8.10}$$

We can therefore obtain a time scale by taking the inverse of the above equation. This is approximately the time it takes for the occupation probability of a state on top of the Fermi surface to change by unity. As in the classical case where a few units of the time between collisions are enough to lead to thermal equilibrium,[32] so it is here that the relaxation time $\tau_{\text{relax}}$ leading to thermal equilibrium is expected to be a few units (say, 5) of the time for a state on top of the Fermi sea to change its occupation probability by unity:

$$\tau_{\text{relax}} \sim 4000/A \text{ fm}/c. \tag{8.11}$$

A dynamical motion is therefore slow or fast depending on whether the time scale involved is much greater or much less than this unit.

## IX. STATIC SOLUTIONS OF THE MASTER EQUATION AT THERMAL EQUILIBRIUM

In the previous section, the concept of thermal equilibrium of a nuclear many-body system has been introduced in terms of stationary occupation numbers. This is a direct consequence of the $H$ theorem which plays a central role in the discussions of irreversible dissipative phenomena. We have seen pictorial examples which illustrate the mechanism and conditions by which a final equilibrium configuration is approached from an initial, nonequilibrium configuration. We wish to study the characteristics of the solutions at thermal equilibrium themselves.

From the $H$ theorem the necessary and sufficient condition for thermal equilibrium is that for any combination of four single-particle levels $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$

$$D(\lambda_1\lambda_2;\lambda_3\lambda_4)[(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4} - n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})] = 0, \tag{9.1}$$

where, in general, the constraint of energy conservation is expressed by $D$, which may be any distribution function peaked at $\epsilon_{\lambda_1}+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4}=0$ and vanishingly small outside a certain neighborhood. In particular, it can be a $\delta$ function or a Lorentzian as the case may be.

### A. Fermi-Dirac distribution as the static solution in an idealized case

We consider first the idealized situation where a $\delta$ function is used for $D$ in Eq. (9.1). Equation (9.1) is then equivalent to a functional relation

$$[1-n(\epsilon_1)][1-n(\epsilon_2)]n(\epsilon_3)n(\epsilon_4) = n(\epsilon_1)n(\epsilon_2)[1-n(\epsilon_3)][1-n(\epsilon_4)], \tag{9.2}$$

under the constraint

$$\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4=0 \tag{9.3}$$

where we have used the abbreviated subscript 1, 2, 3, and 4 to stand for $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$, respectively. It is easy to see that a Fermi-Dirac distribution

$$n(\epsilon) = \frac{1}{1+\exp[(\epsilon-\epsilon_F)/k_BT]}, \tag{9.4}$$

characterized by a temperature $T$ and a Fermi energy $\epsilon_F$, will satisfy Eqs. (9.2) and (9.3). However, one is also interested in studying the converse in the hope of establishing the uniqueness of this type of solution to the number equation.

We assume that the spacing of the single-particle levels is regular enough so that the discrete set $\{n(\epsilon_\lambda)\}$ can be replaced by a smooth distribution function $n(\epsilon)$ $[0<n(\epsilon)<1]$. We then introduce an auxiliary distribution function $y(\epsilon)$, so that

$$n(\epsilon) = \frac{1}{1+y(\epsilon)}. \tag{9.5}$$

It is clear that $0<y(\epsilon)<\infty$. Then Eqs. (9.2) and (9.3) can be re-expressed by a single functional equation

$$y(\epsilon_1)y(\epsilon_2) = y(\epsilon_3)y(\epsilon_1+\epsilon_2-\epsilon_3), \tag{9.6}$$

which is satisfied for independent values of $\epsilon_1$, $\epsilon_2$, and $\epsilon_3$ over a domain of nonzero measure. For any arbitrary but fixed value of $\epsilon_3$, the partial differentiation of Eq. (9.6) with respect to $\epsilon_1$ and $\epsilon_2$ leads to

$$y'(\epsilon_1)y(\epsilon_2) = y(\epsilon_3)y'(\epsilon_1+\epsilon_2-\epsilon_3) \tag{9.7}$$

and

$$y(\epsilon_1)y'(\epsilon_2) = y(\epsilon_3)y'(\epsilon_1+\epsilon_2-\epsilon_3). \tag{9.8}$$

Combining Eqs. (9.7) and (9.8), we have

$$\frac{y'(\epsilon_1)}{y(\epsilon_1)}=\frac{y'(\epsilon_2)}{y(\epsilon_2)}\,. \tag{9.9}$$

Since Eq. (9.9) holds for any $\epsilon_1$ and $\epsilon_2$, it must be equal to a constant, which, in turn, implies that the auxiliary distribution function $y$ must be an exponential function. Now, returning to the original function $n(\epsilon)$, it must have the functional form

$$n(\epsilon)=\frac{1}{1+\exp[\beta(\epsilon-\mu)]}\,, \tag{9.10}$$

for some constants $\beta$ and $\mu$. We note that if we associate $\mu$ with the Fermi energy then $\beta$, the inverse temperature, can only be positive in order to have a reasonable shape of the distribution. We have thus established the uniqueness of solution (9.4) as the static solution for a system in thermal equilibrium in this case.

### B. Static solutions for a discrete system and $\Gamma_\lambda \neq 0$

It should be pointed out that the arguments in the previous paragraphs leading to the uniqueness of the Fermi-Dirac function as the static solution are based on two assumptions. It has been assumed that the spacing of the original discrete single-particle levels is sufficiently regular so that the discrete distribution can be replaced by a continuous function. Furthermore, the single-particle states are assumed to have an infinite lifetime so that the conservation condition is expressed in terms of a δ function. With regard to the first assumption, the restriction should be removed whenever it is possible to do so. The second assumption concerning $\Gamma_i = 0$ needs to be modified if one wants to be self-consistent.

It is easy to see that particles and holes have finite lifetimes due to particle collisions. The master equation can be rewritten in the following form:

$$\frac{\partial n_\lambda}{\partial t}=-P_\lambda^{(-)}n_\lambda+P_\lambda^{(+)}(1-n_\lambda)\,, \tag{9.11}$$

where $P_\lambda^{(-)}$ stands for rate of outgoing probability and $P_\lambda^{(+)}$ for rate of incoming probability. More explicitly, the rates $P_\lambda^{(-)}$ and $P_\lambda^{(+)}$ are given by

$$P_\lambda^{(-)}=\frac{\pi}{\hbar}\sum_{\lambda_2\lambda_3\lambda_4}\delta(\epsilon_\lambda+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4})n_{\lambda_2}(1-n_{\lambda_3})\times(1-n_{\lambda_4})\,|\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle|^2 \tag{9.12}$$

and

$$P_\lambda^{(+)}=\frac{\pi}{\hbar}\sum_{\lambda_2\lambda_3\lambda_4}\delta(\epsilon_\lambda+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4}\times|\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle|^2\,. \tag{9.13}$$

To obtain an approximate time dependence of the occupation numbers, we assume that the rates $P_\lambda^{(+)}$ and $P_\lambda^{(-)}$ are independent of time. In that case, the occupation number of a single-particle state is given by

$$n_\lambda(t)=n_\lambda(t_0)e^{-\Gamma_\lambda(t-t_0)/\hbar}+\frac{\Gamma_\lambda^{(+)}}{\Gamma_\lambda}(1-e^{-\Gamma_\lambda(t-t_0)/\hbar})\,, \tag{9.14}$$

where

$$\Gamma_\lambda=\Gamma_\lambda^{(+)}+\Gamma_\lambda^{(-)} \tag{9.15}$$

and

$$\Gamma_\lambda^{(\pm)}=\hbar P_\lambda^{(\pm)}\,. \tag{9.16}$$

Thus, for short-enough duration for which the second term of (9.14) is very small, the occupation number decreases exponentially with a decay constant of $\hbar/\Gamma_\lambda$. Similarly, the degree of emptiness of a single-particle state $1-n_\lambda$, which appears in the particle Green's function $g^>$, depends on time according to

$$[1-n_\lambda(t)]=[1-n_\lambda(t_0)]e^{-\Gamma_\lambda(t-t_0)/\hbar}+\frac{\Gamma_\lambda^{(-)}}{\Gamma_\lambda}(1-e^{-\Gamma_\lambda(t-t_0)/\hbar})\,. \tag{9.17}$$

Again, for short-enough duration for which the second term of Eq. (9.17) is very small, the degree of emptiness decreases with a decay constant $\hbar/\Gamma_\lambda$.

To provide a correction to the master equation, one is well advised to modify the assumption of Eq. (5.4) by including the time dependence of the occupation probability (9.14) and (9.17). However, to include all the terms in (9.14) and (9.17) will make the problem intractable. Furthermore, for short time intervals where $t-t_0$ is small, the second terms of Eqs. (9.14) and also (9.17) are small. We therefore neglect these terms in approximating the time dependence of the occupation number and the degree of emptiness of the single-particle states, so that the Green's function for the holes is approximately

$$g^<(1,1')\simeq\sum_\lambda n_\lambda(t_1)e^{-\Gamma_\lambda(t_1'-t_1)/2\hbar}\times\psi_\lambda(x_1t_1)\psi_\lambda^*(x_1't_1')\,, \tag{9.18}$$

while the complementary Green's function for the particles is approximately

$$g^>(1,1')\simeq\sum_\lambda[1-n_\lambda(t_1)]e^{-\Gamma_\lambda(t_1'-t_1)/2\hbar}\times\psi_\lambda(x_1t_1)\psi_\lambda^*(x_1't_1')\,. \tag{9.19}$$

As we mentioned before in Sec. VI, when Eqs. (9.18) and (9.19) are substituted, one obtains a master equation which is the same as (6.4), except that the δ function now is modified to become the Lorentzian distribution $D(\epsilon_{\lambda_1}+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4})$ of Eqs. (6.12) and (6.13).

We now return to study the static thermal equilibrium of a discrete system and $\Gamma_\lambda \neq 0$. In such a case, the occupation number is independent of time, so that

$$n_\lambda = \left(\frac{\Gamma_\lambda^{(+)}}{\Gamma_\lambda^{(+)}+\Gamma_\lambda^{(-)}}\right), \tag{9.20}$$

where

$$\Gamma_\lambda^{(+)} = \pi \sum_{\lambda_2\lambda_3\lambda_4} D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4) n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4}) \times |\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle|^2, \tag{9.21}$$

$$\Gamma_\lambda^{(-)} = \pi \sum_{\lambda_2\lambda_3\lambda_4} D(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)(1-n_{\lambda_2}) n_{\lambda_3} n_{\lambda_4} \times |\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle|^2, \tag{9.22}$$

and

$$D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4) = \frac{1}{2\pi}\frac{\Gamma_{1234}}{(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)^2+(\Gamma_{1234}/2)^2}. \tag{9.23}$$

Thus, knowing the energies of the single-particle states and the matrix elements, one can iterate Eqs. (9.20)–(9.23) to obtain the occupation numbers, using a Lagrange multiplier to conserve total particle numbers during iteration. As the widths depend on the occupation numbers in a nonlinear way, the resultant solution should depend on the initial distribution assumed. The class of solutions can therefore be classified by the parameters which specify the initial distribution. For example, one may use the parameter of a temperature to characterize both the initial distribution and also the resultant distribution after iterations. The case of zero temperature ($T = 0$) ground state occupation number distribution has been studied by Orland and Schaeffer.[47] Other cases have, however, not been studied.

Before we close this section, we should note in passing that the widths $\Gamma_\lambda$ as we discuss in this static thermal equilibrium are due only to particle collisions. In the general case when there is also dynamical motion, the widths are not just due to collision alone but also to the dynamical motion of the mean field. The latter width, which we call the dynamical width $\Gamma_\lambda^{(d)}$, is approximately

$$\Gamma_\lambda = 2[\langle\psi_\lambda, (h-\epsilon_\lambda)^2\psi_\lambda\rangle]^{1/2}.$$

Thus, in the general case, the total width $\Gamma_\lambda$ is

$$\Gamma_\lambda = \Gamma_\lambda^{(d)} + \Gamma_\lambda^{(+)} + \Gamma_\lambda^{(-)},$$

and the Lorentzian of Eq. (6.13) is defined with respect to this total width.

## X. MACROSCOPIC EQUATIONS IN DENSITY AND CURRENT AND THE CORRESPONDING CONSERVATION LAWS

It is well known that macroscopic equations can be systematically obtained from the equations of the Green's functions by taking appropriate moments and limits. These equations contain useful information about the time development of the macroscopic dynamical variables of the system. With the incorporation of particle collisions in ETDHF, the corresponding macroscopic equations—the equation of continuity, the Euler-type equation for momentum density, and the equation of energy density—can be obtained to provide a clear picture of how microscopic and macroscopic degrees of freedom are coupled via the mechanism of particle collisions. In general, these equations contain terms which are the same as those obtained in the TDHF theory, with the exception that the time-dependent occupation numbers for the single-particle states need to be accounted for. There are new contributions, however, which arise from the additional collision matrix.

To obtain the macroscopic equations, it is convenient to start with the equation of the one-body density matrix which is the equal-time limit of Eq. (2.15),

$$\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}(\nabla_x{}^2-\nabla_{x'}{}^2)-U_{\mathrm{MHF}}(xt)+U_{\mathrm{MHF}}(x't)\right) \times \mathfrak{N}(x,x';) = -iI(x,x';t), \tag{10.1}$$

where the collision matrix $I$ is given by Eq. (5.6) explicitly in terms of occupation numbers and the microscopic single-particle wave functions. In the following discussion, our attention will be focused on the new contributions to the macroscopic equation introduced by the collision matrix. The derivations of the rest of the terms are essentially the same as presented in some earlier work (Refs. 1–3) and will not be repeated here.

### A. Equation of continuity and total particle number conservation

The equation of motion for the density field is obtained by taking the limit $x' \to x$ in Eq. (10.1). From Eq. (5.5), it is clear that

$$\lim_{x'\to x} I(x,x';t) = 0, \tag{10.2}$$

and hence the collision matrix gives no contribution to the equation of continuity. This result remains valid even when the $\delta$ function in the master equation is replaced by a distribution $D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ symmetrical with respect to the interchange of $\epsilon_1 \rightleftarrows \epsilon_4$ and $\epsilon_2 \rightleftarrows \epsilon_3$, such as the Lorentzian form of Eq. (6.12).

The usual continuity equation as given by Eq. (5.4) of Ref. 2 is then preserved in a trivial manner. In particular, in the presence of zero range exchange interactions, we have

$$\frac{\partial \rho(x,t)}{\partial t} + \nabla \cdot \vec{J}(x,t) = 0\,, \qquad (10.3)$$

where, for ETDHF, the number density field and the current field are defined by

$$\rho(x,t) = \sum_{\lambda} n_{\lambda}(t)\psi_{\lambda}(xt)\psi_{\lambda}^{*}(xt) \qquad (10.4)$$

and

$$\vec{J}(xt) = \sum_{\lambda} n_{\lambda}(t)\vec{J}_{\lambda}(xt)\,, \qquad (10.5)$$

with $\vec{J}_{\lambda}$, the local current density due to the modified TDHF state $\lambda$, defined in the usual way:

$$\vec{J}_{\lambda}(xt) = \frac{\hbar}{2mi}\left[\psi_{\lambda}^{*}(xt)\nabla\psi_{\lambda}(xt) - \nabla\psi_{\lambda}^{*}(xt)\psi_{\lambda}(xt)\right]. \qquad (10.6)$$

Accordingly, the velocity field $\vec{u}$ can be defined as

$$\vec{u}(x,t) = \vec{J}(xt)/\rho(xt)\,. \qquad (10.7)$$

The total particle number is obtained from the density field as follows:

$$N_{\text{tot}}(t) = \int dx\,\rho(x,t)\,. \qquad (10.8)$$

The conservation of total particle number is easily obtained by an integration of Eq. (10.3) over all space and an application of the master equation.

It should be noted that we have assumed a zero-range exchange interaction for the density-dependent part of the effective interaction. In the case where there is a non-zero-range exchange component, we shall have an additional source term on the right-hand side of the continuity equation (10.3).[2] But the conservation of total particle numbers is still valid and can be readily seen from Eq. (6.4). Hence, the presence of the additional source term associated with exchange of particles at different locations globally does not affect the conservation of the total particle number.

### B. Euler equation and total momentum conservation

The vector equation of the momentum density flux is obtained by taking the limit of $\vec{r}' \to \vec{r}$ after operating $(\nabla_r - \nabla_{r'})$ onto Eq. (10.1). In component form, this is given by

$$\frac{\partial(m\rho u_i)}{\partial t} + \sum_{j=1}^{3} \nabla_j\left(\rho u_i u_j + p_{ij}^{(q)} + p_{ij}^{(t)}\right) = -\int dx'\,\nabla_i v(x,x')\left[\mathfrak{N}(x',x';t)\mathfrak{N}(x,x;t) - \mathfrak{N}(x,x';t)\mathfrak{N}(x',x;t)\right] + F_i^{(c)}(x,t)\,, \qquad (10.9)$$

where $p_{ij}^{(q)}$ and $p_{ij}^{(t)}$ are the generalized quantum and thermal stress tensors, respectively,

$$p_{ij}^{(q)}(x,t) = \sum_{\lambda} n_{\lambda}(t) p_{ij;\lambda}^{(q)}(x,t)\,, \qquad (10.10)$$

$$p_{ij}^{(t)}(x,t) = \sum_{\lambda} n_{\lambda}(t) p_{ij;\lambda}^{(t)}(x,t)\,. \qquad (10.11)$$

These stress tensors are obtained by summing over components due to various single-particle states,[3] that is,

$$p_{ij;\lambda}^{(q)}(x,t) = \left(-\frac{\hbar^2}{4m}\nabla_i\nabla_j\phi_{\alpha}{}^2(\vec{r},t) + \frac{\hbar^2}{m}\nabla_i\phi_{\alpha}(\vec{r},t)\nabla_j\phi_{\alpha}(\vec{r},t)\right)\Xi_{\sigma}(\xi)\Xi_{\sigma}^{\dagger}(\xi)\,, \qquad (10.12)$$

$$p_{ij;\lambda}^{(t)}(x,t) = \left[m\phi_{\alpha}{}^2(\nabla_i S_{\alpha} - u_i)(\nabla_j S_{\alpha} - u_j)\right]\Xi_{\sigma}(\xi)\Xi_{\sigma}^{\dagger}(\xi)\,, \qquad (10.13)$$

where the spatial part of the single-particle wave functions are rewritten in the polar form,[3]

$$\psi_{\lambda}(x,t) = \phi_{\lambda}(\vec{r},t)\exp[imS_{\lambda}(\vec{r},t)/\hbar]\,\Xi_{\sigma}(\xi)\,. \qquad (10.14)$$

The first term on the right-hand side of the Euler equation (10.9) represents the force density arising from the mean field. It has the form of folding of the two-body force with the uncorrelated part of the two-body distribution function $i^2 g_{20}(xt,x't;xt^+,x't^+)$ represented by quantities in the square brackets. As the two-body distribution function gives the probability for finding a particle at position $x'$ when another particle is at $x$, such a force density term has a simple physical interpretation.

The additional force term $F_i^{(c)}$ is due to the presence of particle collisions. In vector form, it is related to the collision matrix as

$$\vec{F}^{(c)}(xt)=\tfrac{1}{2}i\lim_{x'\to x}\left[(\nabla_r-\nabla_{r'})I(x,x';t)\right]. \tag{10.15}$$

From the expression given in (5.6), after some straightforward calculation, $\vec{F}^{(c)}$ can be written in terms of single-particle wave functions,

$$\begin{aligned}\vec{F}^{(c)}(x,t)=\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}&[\epsilon_{\lambda_1}+\epsilon_{\lambda_2}-\epsilon_{\lambda_3}-\epsilon_{\lambda_4}-i\eta]^{-1}_{\eta\to 0}[(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4}-n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})]\\&\times\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle\int dx''\,\nabla v'(x,x'')\psi_{\lambda_1}(xt)\psi_{\lambda_2}(x''t)\psi^*_{\lambda_3}(x''t)\psi^*_{\lambda_4}(xt).\end{aligned} \tag{10.16}$$

This force density arises from particle collisions. It can be shown to be the folding of the two-body residual force with the correlation part of the two-body distribution function $i^2 g_{2c}(xt,x't;xt^+,x't^+)$, as expected.

The conservation of momentum associated with the Euler equation can be directly obtained by integrating over $\vec{r}$. With a conservative two-body force which depends on the relative spatial coordinates, the contributions from the force densities arising from the mean field and the residual interaction vanish. We have

$$\frac{\partial}{\partial t}\int dx\,\rho\vec{u}=0, \tag{10.17}$$

and thus the total momentum of the system is conserved. This result remains valid even when the δ function in the master equation is replaced by a distribution $D(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$ symmetric with respect to the interchange of $\epsilon_1\rightleftharpoons\epsilon_4$ and $\epsilon_2\rightleftharpoons\epsilon_3$.

## XI. MACROSCOPIC EQUATION OF ENERGY DENSITY AND THE CONSERVATION OF TOTAL ENERGY

The equation for energy density can be directly obtained from Eq. (10.1) by taking the limit $\vec{r}'\to\vec{r}$ after operating $\nabla_r\cdot\nabla_{r'}$ onto Eq. (10.1). We then obtain the following equation which is a generalization of the corresponding TDHF energy equation given in Eq. (3.30) of Ref. 3:

$$\begin{aligned}\frac{\partial}{\partial t}[\rho E_k]+\sum_{i=1}^{3}\nabla_i\Big(\rho E_k u_i+\sum_{j=1}^{3}(p_{ij}^{(q)}+p_{ij}^{(t)})u_j+F_i\Big)&\\=-\int dx''\sum_{i=1}^{3}\Big(\rho(x,t)\rho(x'',t)u_i(x'',t)-\frac{\hbar}{m}\mathrm{Im}\,\mathfrak{N}(x'',x;t)\nabla_i\mathfrak{N}(x,x'';t)\Big)&\nabla_i v(x,x'')+P_I(x,t),\end{aligned} \tag{11.1}$$

where the generalized kinetic energy density is given by

$$\begin{aligned}E_k(xt)&=\frac{\hbar^2}{2m}\sum_\lambda n_\lambda(t)\nabla\psi^*_\lambda(xt)\cdot\nabla\psi_\lambda(xt)/\rho(xt)\\&=\sum_\lambda n_\lambda[\tfrac{1}{2}m\phi_\lambda{}^2(\nabla S_\lambda)^2+(\hbar^2/2m)(\nabla\phi_\lambda)^2]/\rho.\end{aligned} \tag{11.2}$$

and the generalized heat flux density is given by

$$\begin{aligned}F_i(xt)=\sum_\lambda n_\lambda\Big[&\Big(\frac{1}{2}m\phi_\lambda{}^2(\nabla S_\lambda)^2+\frac{\hbar^2}{2m}(\nabla\phi_\lambda)^2\Big)(\nabla_i S_\lambda-u_i)\\&+\sum_{j=1}^{3}\Big(-\frac{\hbar^2}{4m}\nabla_i\nabla_j\phi_\lambda{}^2+\frac{\hbar^2}{m}\nabla_i\phi_\lambda\nabla_j\phi_\lambda\Big)(\nabla_j S_\lambda-u_j)+\frac{\hbar^2}{2m}\phi_\lambda\nabla_i\phi_\lambda\nabla^2 S_\lambda\Big].\end{aligned} \tag{11.3}$$

Equation (11.1) in form corresponds exactly to Eq. (3.30) of Ref. 3, except that on the right-hand side there is an additional density term $P_I$ which is due to particle collisions. It is obtained either from the collision matrix or the correlated part of the two-body Green's function as follows:

$$P_I(x,t) = -\frac{\hbar}{2m} \lim_{x' \to x} [(\nabla_r \cdot \nabla_{r'}) I(x,x';t)] . \tag{11.4}$$

This additional term gives the rate of change of the local energy density due to the residual interaction. From the expressions of $I$ or $g_{2c}$ given previously, $P_I$ can be explicitly written down in terms of occupation numbers and the single-particle basis states:

$$P_I(x,t) = \frac{\hbar}{2im} \sum_{1234} \left( \frac{1}{\epsilon_1 + \epsilon_2 - \epsilon_3 - \epsilon_4 - i\eta} \right)_{\eta \to 0} [(1-n_1)(1-n_2)n_3n_4 - n_1n_2(1-n_3)(1-n_4)] \langle 12 | v' | 43 - 34 \rangle$$
$$\times \int dx'' [\nabla \psi_1(x,t) \psi_2(x'',t) \psi_3^*(x'',t) \psi_4(x,t) - \psi_1(x,t)\psi_2(x'',t)\psi_3^*(x'',t) \nabla \psi_4^*(x,t)] \cdot \nabla v'(x,x'') . \tag{11.5}$$

As one can see, the final form is somewhat complicated. It will be of interest in future work to investigate if there are dynamical conditions under which this may be approximated in a simple way in terms of local dynamical variables.

We turn now to the discussion of the conservation of the total energy in ETDHF, we shall study the slightly more general case where the correlated part of the two-body Green's function $g_{2c}$ is given by a perturbation expansion up to the first order in $v'$ [Eq. (3.14)]. This will set up the framework for a subsequent discussion where one further invokes the next level of slow mean-field approximation.

An operation of $-(\hbar/2m)\lim_{1' \to 1}(\nabla_{r_1} \cdot \nabla_{r'_1})$ onto Eq. (3.12) of the one-body Green's function, and a subsequent integration over the coordinate $x$, leads to the following without any approximations:

$$\frac{\partial}{\partial t_1} \int dx_1 T(x_1,t_1) + \frac{\hbar}{2im} \int dx_1 dx_2 [v(x_1,x_2) \lim_{1' \to 1} ({\nabla_{r_1}}^2 - {\nabla_{r'_1}}^2) g_{20}(12;1'2^+)$$
$$+ v'(x_1.x_2) \lim_{1' \to 1} ({\nabla_{r_1}}^2 - {\nabla_{r'_1}}^2) g_{2c}(12;1'2^+)] = 0 , \tag{11.6}$$

where the kinetic energy density $T$ is given by

$$T(x,t) = \frac{\hbar^2}{2im} \lim_{x' \to x} \nabla_r \cdot \nabla_{r'} \, g(xt;x't^+) = \frac{\hbar^2}{2m} \sum_\lambda n_\lambda(t) \nabla \psi_\lambda^*(xt) \cdot \nabla \psi_\lambda(xt) . \tag{11.7}$$

From the perturbation expansion of $g_{2c}$[Eq. (3.14)], Eq. (11.6) can be finally simplified to become the following:

$$\frac{\partial}{\partial t_1} \left( \int T(x_1 t_1) dx_1 + \tfrac{1}{2} \int dx_1 dx_2 \, [v(x_1,x_2) i^2 g_{20}(12;1^+2^+) + v'(x_1,x_2) i^2 g_{2c}(12;1^+2^+)] \right) = 0 . \tag{11.8}$$

We can now define a total energy for ETDHF,

$$E_{\text{tot}} = \int dx_1 \left( T(x,t) + \tfrac{1}{2} \int dx_2 [v(x_1,x_2) i^2 g_{20}(12;1^+2^+) + v'(x_1,x_2) i^2 g_{2c}(12;1^+2^+)] \right) , \tag{11.9}$$

which, as can be readily seen from Eq. (11.8), is conserved. The terms in Eq. (11.9) have simple physical meaning. The first term is the total kinetic energy. As $i^2 g_{20}(12, 1^+2^+)$ is the two-body distribution function without the correlation due to particle collision, the second term is the interaction energy due to the uncorrelated part of the two-body distribution function. The third term is the correlated interaction energy due to particle collisions.

Now we consider the next level of approximation with a slow mean field. The correlated part of the two-body Green's function and the collision matrix are now in the Markovian form. A direct evaluation of the operation $\nabla_r \cdot \nabla_{r'}$ on the collision matrix of Eq. (5.6) leads to the following:

$$-\frac{\hbar}{2m} \int dx \lim_{x' \to x} \nabla_r \cdot \nabla_{r'} I(x;x';t) = \tfrac{1}{4} \sum_{1234} \left( \frac{1}{\epsilon_1 + \epsilon_2 - \epsilon_3 - \epsilon_4 - i\eta} \right)_{\eta \to 0} [(1-n_1)(1-n_2)n_3n_4 - n_1n_2(1-n_3)(1-n_4)]$$
$$\times \langle 12 | v' | 43 - 34 \rangle \frac{\partial}{\partial t} \langle 43 - 34 | v' | 12 \rangle . \tag{11.10}$$

We wish to cast the above result into the form of (11.8), which is what one expects intuitively. Such a manipulation introduces new correction terms to the right-hand side of (11.8). We have, for this level of approximation, the energy conservation law expressed in the following form:

$$\frac{\partial}{\partial t}\left(\int T(x_1)dx_1+\tfrac{1}{2}\int dx_1dx_2[v(x_1,x_2)i^2g_{20}(12,1^+2^+)+v'(x,x_2)i^2g_{2c}(12,1^+2^+)]\right)_{t_1=t_2}=\Theta_1'+\Theta_2', \tag{11.11}$$

where $g_{2c}(12,1^+2^+)$ is in the Markovian form as given by Eq. (5.5).

In terms of the matrix elements and occupation numbers, the contribution to the total energy involving $g_{2c}$ is explicitly

$$\tfrac{1}{2}\int dx_1dx_2v'(x_1,x_2)i^2g_{2c}(12,1^+2^+)_{t_1=t_2}=\tfrac{1}{4}\sum_{1234}n_1n_2(1-n_3)(1-n_4)\mathcal{P}\left(\frac{1}{\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4}\right)|\langle 12|v'|43-34\rangle|^2, \tag{11.12}$$

where $\mathcal{P}$ denotes the principal value. It has the form of what one expects from a second-order perturbation theory. In Eq. (11.11), the new correction terms are

$$\Theta_1'=\tfrac{1}{4}\sum_{1234}\frac{\partial}{\partial t}\left[(n_1n_2(1-n_3)(1-n_4)\mathcal{P}\left(\frac{1}{\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4}\right)\right]|\langle 12|v'|43-34\rangle|^2 \tag{11.13}$$

and

$$\Theta_2'=\frac{-\pi i}{4}\sum_{1234}n_1n_2(1-n_3)(1-n_4)\delta(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)$$
$$\times\left(\langle 12|v'|43-34\rangle\frac{\partial}{\partial t}\langle 43-34|v'|12\rangle-\langle 43-34|v'|12\rangle\frac{\partial}{\partial t}\langle 12|v'|43-34\rangle\right). \tag{11.14}$$

The correction term $\Theta_1'$ is a measure of the error in assuming the slow variation of $n_\lambda$ and $\epsilon_\lambda$ in Eqs. (5.3) and (5.4). The correction term $\Theta_2'$ is a measure of the error in using the approximation (5.1) for the temporal variation of the wave function. If the temporal variation is indeed given by (5.1), this term vanishes when the energy conservation is expressed by a $\delta$ function but assumes a finite value when the $\delta$ function in energy is replaced by a Lorentzian

$$\Theta_2'=-\frac{\pi}{2\hbar}\sum_{1234}n_1n_2(1-n_3)(1-n_4)\frac{(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)\Gamma_{1234}/2}{(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)^2+(\Gamma_{1234}/2)^2}|\langle 12|v'|43-34\rangle|^2. \tag{11.15}$$

Such correction terms may be of practical interest in the actual numerical implementation of ETDHF in the future. Except for these corrections which arise from the slow mean-field approximation and the absence of a width, the total energy as given by Eqs. (11.9) and (11.11) is conserved.

The foregoing discussion concerning the conservation of total energy indicates the need for further investigation. There are many ways to address this problem. One can try to obtain a variational principle in such a way that the resultant equations of motion are essentially those obtained there. In the process, the total energy can be made conserved by the use of Lagrange multipliers. Another method makes a more general parametrization of the occupation probability as

$$n_\lambda(t_1,t_2)=n_\lambda\left(\frac{t_1+t_2}{2}\right)\frac{\exp[-(t_1-t_2)^2/2S_\lambda^2]}{\sqrt{2\pi}\,S_\lambda}. \tag{11.16}$$

Or, in the Fourier space, the occupation is parametrized as a function of $p$ and $\omega$.[7] We present below a different method with a limited objective of conserving only the energy defined by

$$E=\int dxT(x,t)+\tfrac{1}{2}\int dx_1dx_2v(x_1,x_2)i^2g_{20}(x_1t,x_2t;x_1t,x_2t). \tag{11.17}$$

That is, $E$ is the total energy as calculated only with the mean field but neglecting the correlation energies due to $g_{2c}$. For such a purpose, we note that our equation of motion, because of the assumption concerning the off-diagonal matrix elements of the occupation matrix $n_{\lambda\lambda'}$, is essentially

$$i\hbar\frac{\partial}{\partial t}g^{<}(1,1')_{t_1'=t_1=t}+\left(\frac{\hbar^2}{2m}(\nabla_1{}^2-\nabla_{1'}{}^2)-U_{\mathrm{MHF}}(1)+U_{\mathrm{MHF}}(1')\right)g^{<}(1,1')_{t_1'=t_1=t}=-\hbar\sum_{\lambda}\left(\frac{\partial}{\partial t}n_\lambda\right)[\psi_\lambda(1)\psi_\lambda^*(1')]_{t_1'=t_1=t}\,. \tag{11.18}$$

One can show from the above that

$$\frac{\partial}{\partial t}E=\sum_{\lambda}\frac{\partial n_\lambda}{\partial t}\epsilon_\lambda\,. \tag{11.19}$$

The energy as defined by Eq. (11.17) is conserved if the right-hand side of Eq. (11.19) is made zero. This can be achieved with the introduction of an energy shift $\delta\epsilon$ for each single-particle state.[48] Specifically, we parametrize the Green's functions by

$$g^{<}(1,1')=\sum_{\lambda}n_\lambda\left(\frac{t_1+t_1'}{2}\right)\exp[-i\delta\epsilon_\lambda(t_1-t_1')/\hbar]\psi_\lambda(1)\psi_\lambda^*(1') \tag{11.20}$$

and, similarly,

$$g^{>}(1,1')=\sum_{\lambda}\left[1-n_\lambda\left(\frac{t_1+t_1'}{2}\right)\right]\exp[-i\delta\epsilon_\lambda(t_1-t_1')/\hbar]\psi_\lambda(1)\psi_\lambda^*(1')\,. \tag{11.21}$$

This parametrization preserves all the equal-time properties of the Green's functions while exploiting the unequal-time Green's functions in a new way. If we modify our single-particle Hamiltonian in the following manner,

$$i\hbar\frac{\partial}{\partial t}\psi_\lambda(x,t)=\left(-\frac{\hbar^2}{2m}\nabla^2+U_{\mathrm{MHF}}(x,t)-\delta\epsilon_\lambda(t)\right)\psi_\lambda(x,t)\,, \tag{11.22}$$

while maintaining

$$\epsilon_\lambda(t)=\langle\psi_\lambda(xt),[-(\hbar^2/2m)\nabla^2+U_{\mathrm{MHF}}(xt)]\psi_\lambda(xt)\rangle\,, \tag{11.23}$$

then the master equation is obtained in the same form as Eqs. (5.8) and (6.12), except now the Lorentzian is given by

$$D(\epsilon_1,\epsilon_2,\epsilon_3,\epsilon_4)=\frac{1}{2\pi}\frac{\Gamma_{1234}}{(\epsilon_1+\delta\epsilon_1+\epsilon_2+\delta\epsilon_2-\epsilon_3-\delta\epsilon_3-\epsilon_4-\delta\epsilon_4)^2+(\Gamma_{1234}/2)^2}\,. \tag{11.24}$$

The right-hand side of Eq. (11.22) can be made equal to zero if $\delta\epsilon_\lambda$ is so chosen that

$$\delta\epsilon_\lambda=-\epsilon_\lambda\frac{\Gamma_\lambda^{(+)}(1-n_\lambda)-\Gamma_\lambda^{(-)}n_\lambda}{2[\Gamma_\lambda^{(+)}(1-n_\lambda)-\Gamma_\lambda^{(-)}n_\lambda-\mathcal{P}_\lambda]}\,, \tag{11.25}$$

where

$$\mathcal{P}_\lambda=\frac{\hbar}{8\pi}\sum_{234}\frac{\Gamma_{\lambda 234}{}^2|\langle\lambda 2|v'|43-34\rangle|^2}{[(\epsilon_\lambda+\epsilon_2-\epsilon_3-\epsilon_4)^2+(\Gamma_{\lambda 234}/2)^2]^2}[(1-n_\lambda)(1-n_2)n_3n_4-n_\lambda n_2(1-n_3)(1-n_4)]\,. \tag{11.26}$$

Thus, by a proper shift of the single-particle energies, the total energy as defined by Eq. (11.17) can be made to conserve. Whether such a simple scheme can be made practical remains to be further investigated.

## XII. MANY-BODY INFORMATION FROM ETDHF APPROXIMATION

With the time-dependent Hartree-Fock approximation, we have a many-body wave function in the form of a single Slater determinant, if it is initially a determinant. It is remarkable that this can be the case in view of the fact that only a one-body density matrix is determined here. The transcription from a one-body density to a many-body wave function is possible because of conservation of the idempotent property which, together with normalization and symmetry properties, determines uniquely a Slater determinant (up to a unitary transformation) (Appendix A).

What does the idempotent property become in the presence of particle collisions? We can use the normalization condition for the two-body density matrix $\mathfrak{N}_2$

$$(A-1)\mathfrak{N}(x_1,x_1';t)=\int dx_2\mathfrak{N}_2(x_1x_2,x_1'x_2;t)\,, \tag{12.1}$$

and we obtain

$$\mathfrak{N}(x_1,x_1';t)=+\int dx_2\mathfrak{N}(x_1,x_2;t)\mathfrak{N}(x_2,x_1';t)+\int dx_2 g_{2c}(12,1'2^+)_{\substack{t_1'=t_1^+\\ t_1=t_2}}\,. \tag{12.2}$$

Thus, the idempotent property is modified by correlations due to particle collisions and cannot be of direct use to provide many-body information for our case.

We would like to pose our question in a different way. We wish to seek the *simplest* kind of many-body wave function which contains the same one-body and two-body information and into which the system evolves continuously. The requirement on simplicity restricts our choice to the set of determinants $\psi_k$ formed by the set of ETDHF single-particle states $\psi_\lambda(x,t)$

$$\Psi_k(x_1,\ldots,x_A,t)=\mathfrak{a}[\psi_{\lambda_1}(x_1,t)\psi_{\lambda_2}(x_2,t)\cdots\psi_{\lambda_A}(x_A,t)]\,, \tag{12.3}$$

where $\mathfrak{a}$ is the antisymmetrization operator. In Fock space, we represent the determinantal many-particle state $\Psi_k$ by a set of occupation numbers $\nu_{k\lambda}$ such that

$$\begin{aligned}&\nu_{k\lambda}=1 \text{ if state } \lambda \text{ is occupied for the state } \Psi_k\\ &\text{and}\\ &\nu_{k\lambda}=0 \text{ if state } \lambda \text{ is unoccupied}\,.\end{aligned} \tag{12.4}$$

We seek a representation of our many-body system by a wave function as a linear combination of the (known) determinants $\Psi_k$

$$\Psi(x_1,x_2,\ldots,x_A,t)=\sum_k a_k(t)\Psi_k(x_1,x_2,\ldots,x_A,t)\,, \tag{12.5}$$

where the amplitude $a_k$ depends on time. The requirement that this wave function contains the same one-body information leads to

$$\sum_k |a_k(t)|^2\nu_{k\lambda}=n_\lambda\,. \tag{12.6}$$

The requirement that this wave function gives the same two-body distribution function leads to

$$\sum_{kk'} a_k(t)a_{k'}^*(t)\nu_{k\lambda_1}\nu_{k\lambda_2}\nu_{k'\lambda_3}\nu_{k'\lambda_4}D_{kk'}$$
$$=n_{\lambda_1}n_{\lambda_2}\delta_{\lambda_1\lambda_4}\delta_{\lambda_2\lambda_3}+[n_{\lambda_1}n_{\lambda_2}(1-n_{\lambda_3})(1-n_{\lambda_4})-(1-n_{\lambda_1})(1-n_{\lambda_2})n_{\lambda_3}n_{\lambda_4}](\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4-i\eta)^{-1}_{\eta\to 0}\langle 12|v'|43-34\rangle\,,$$

where $D_{kk'}$ equals unity if the set of occupied single-particle states in $\Psi_k$ (besides $\lambda_1$ and $\lambda_2$) are the same as the set in $\Psi_{k'}$ (besides $\lambda_3$ and $\lambda_4$), and $D_{kk'}$ vanishes otherwise. As the right-hand side of Eq. (12.5) and also Eq. (12.6) are known quantities at every instant of time in a dynamical calculation while the occupation numbers for the determinants are also known, one can invert Eqs. (12.5) and (12.6) for a truncated set of determinants to obtain the time dependence of the amplitude $a_k$. When this is carried out successfully, the resultant many-body wave function will provide information on the dynamics of the system, much as the single determinantal wave function does for the TDHF approximation. The many-body information obtained therefrom is, however, deficient. It deficiency will be discussed in the next section.

## XIII. SUMMARY AND DISCUSSIONS

Motivated by the need to extend the TDHF approximation to include particle collision both as a way to study the approach to thermal equilibrium and also to assess the validity of the TDHF approximation, we first obtain the relation between the TDHF approximation and the exact many-body theory. We begin to understand the TDHF approximation as the lowest and simplest truncation of a hierarchy of equations, the so-called Martin-Schwinger hierarchy involving Green's functions.

Such an understanding brings with it a natural way to extend the TDHF approximation to higher orders by truncating the hierarchy at higher levels. When this is carried out, we obtain the correlated part of the two-body Green's function due to particle collisions expressed in terms of a time integral of one-body Green's functions over the past collision history. Such a non-Markovian form is computationally impractical. To convert the collision matrix into a Markovian form, it is necessary to integrate the collision history analytically. This can be carried out when the mean field is varying slowly.

While the Green's function is used to formulate the central problem, for practical purposes, it is convenient to project the Green's function in terms of a complete set of time-dependent single-particle states and their occupation probabilities. The choice of these states to be solutions of a time-dependent modified Hartree-Fock single-particle equation gives a clean separation between the effect of the mean field and the effect of particle collisions. The master equation for the occupation probability in Markovian form is obtained when the mean field is varying slowly. It describes properly the collision process and takes due account of the transition probability, energy conservation, and Pauli exclusion principle. The set of time-dependent equations for the single-particle wave functions [Eq. (6.1) and the master equation for the occupation probability Eq. (6.4)] constitutes the extended time-dependent Hartree-Fock approximation and is the most important result of the present paper.

We proceed next to discuss the implications of the the ETDHF approximation on nuclear dynamics. The occurrence of a $\delta$ function restricting the equality of the two-particle energy levels (or near equality when the width of a single-particle state is allowed) in the master equation leads to the concept of level crossing in our discussion of the collision process. These crossings of levels are made possible by the dynamical motion of the system which changes the mean field and the kinetic energies of the particles. Whenever a level crossing takes place, an energy-conserving collision can proceed to redistribute the occupation probabilities. Remarkably, how the occupation probabilities redistribute themselves can be given by analytic formulas which are obtained here for the first time. The parameter $G^2$ which appears in the analytic formulas has the same meaning as the same parameter in the Landau-Zener formula, but the solutions for slow motion or large interaction are drastically different. The tendency in such cases is to leave the occupation probabilities nearly evenly divided. The redistribution of the occupation probabilities in such a manner leads eventually to thermal equilibrium. In fact, upon introducing entropy in the usual way, one obtains from the master equation the well-known $H$ theorem that entropy never decreases with time. Entropy becomes stationary when the system attains thermal equilibrium characterized by stationary occupation probabilities in the form of a Fermi-Dirac distribution with a temperature (or some modified form when a width is allowed). Thus, with the ETDHF approximation, how a system approaches thermal equilibrium can be simply followed step by step. Specifically, at every time step, one calculates the entropy and measures whether the rate of change of the entropy is leveling off or not. If it is, one makes use of the distribution of the occupation probabilities to extract the temperature.

Our equation of motion in density matrix form is a configuration-space analog of the quantum Boltzman equation. Equations of motion for macroscropic variables and the conservation laws can be simply obtained by taking the proper moments of our equation of motion. We find that the equation of continuity is preserved, and that the equation of momentum and energy contain additional terms due to the correlation coming from particle collisions. These macroscopic equations are not of much practical interest at present, but can be useful as a starting point for future investigations in search of proper simplifying approximations to reduce terms involving microscopic variables into terms involving only macroscopic variables. For example, one can follow a procedure similar to that of Chapman and Enskog[49] to obtain viscosity and thermal conductivity out of our equations of motion for a system near equilibrium.

Along with the macroscopic equations of motion, we also obtain the conservation laws. We can prove that the total number of particles is rigorously conserved and that the total momentum is also rigorously conserved. With regard to the conservation of total energy, we discuss the two different levels of approximation which enter into our formulation. In the first level in which the correlated two-body Green's function is in the non-Markovian form involving a time integration of past history of one-body Green's functions, the total energy is conserved. In the next level of approximation, one invokes further the slow mean field to reduce the non-Markovian correlated two-body Green's function to Markovian form; therefore, the total energy is conserved subject to the restriction on the slowness of the mean field. Whether some of the correction terms can be improved upon is a subject worthy of further investigation in the future. For example, with the introduction of shifts of single-particle energies, the total energy including only the mean field potentials can be made to conserve.

Just as a many-body wave function can be extracted from the TDHF approximation, so it can also be from the ETDHF approximation where a many-body wave function can be extracted from the knowledge of the occupation probabilities and the correlated two-body Green's function. However, it needs to be pointed out that much of this many-body information is deficient in some respects. For example, in the TDHF many-body wave function, information concerning the one-body quantities depends on the dynamics, but information concerning the two- and higher-body quantities is obtained purely from this one-body quantity, with proper allowance only for the correlation effect due to statistics of particles and not to the many-particle interactions. In fact, in the TDHF approximation, a reduced $s$-body density matrix (for $s=2,\ldots,A$) is given in terms of the one-body density matrix by

$$\mathfrak{N}_0^{(s)}(123\cdots s;1'2'3'\cdots s')=\mathfrak{A}[[\cdots\mathfrak{A}[\mathfrak{A}[\mathfrak{N}(1,1')\mathfrak{N}(2,2')]\mathfrak{N}(3,3')]\cdots]\mathfrak{N}(s,s')]\,, \tag{13.1}$$

where $\mathfrak{A}$ is the antisymmetrization operator. Similarly, in the ETDHF approximation, a reduced $s$-body density matrix is given in terms of the one-body and the correlated two-body density matrix $i^2g_{2c}$ by

$$\begin{aligned}\mathfrak{N}^{(s)}(123\cdots s;1'2'3'\cdots s')=\mathfrak{N}_0^{(s)}(123\cdots s;1'2'3'\cdots s')\\ +\sum_{r,u}\mathfrak{A}[\{i^2g_{2c}(ru,r'u')\Big|_{\substack{t'_r=t_t\\ t'_u=t_u\\ t_r=t_u}}\}\mathfrak{N}_0^{(s-2)}(12\cdots r-1\;r+1\cdots u-1\;u+1\cdots s;1'2'\cdots r'-1\\ \times r'+1\cdots u'-1\;u'+1\cdots s')]\,,\end{aligned} \tag{13.2}$$

where $\mathfrak{N}_0^{(s)}$ is given by (13.1) and $s=3,\ldots,A$. Thus, in using the ETDHF many-body density matrix or wave functions for the discussion of three- and higher-body clusters, one should keep in mind that only the correlation effects due to the fermion statistics and two-body correlations are included and that there is the deficiency in neglecting three- and higher-body correlations due to interactions.

We would like to turn now to the question on the validity of TDHF for nuclear dynamics, which is an important question in view of the large number of calculations employing the TDHF approximation. Clearly, how good the TDHF approximation is depends on the correction to the TDHF approximation. The smaller the correction, the better is the approximation. This correction is embodied in our ETDHF approximation. The correction term, which we call collision matrix, gives rise to temporal variations of the occupation probabilities. The question on the validity of TDHF can therefore be put in the form whether the occupation probabilities, which are frozen in the TDHF, undergo large changes. Therefore, based on our results expressed in Eqs. (8.8) and (8.10), and the level crossing formulas, we obtain the comparison of the circumstances in which the TDHF approximation is applicable to those when the collision term is important as shown in Table I. Here the time scale is called short or long depending on its comparison with the unit of $\tau_{\text{relax}}$ given in (8.11). Along with the time scale $\tau_{\text{relax}}$, one can obtain a length scale by multiplying it with a typical velocity. The dimension of the system is called small or large depending on its comparison with this length scale. A motion is called rapid or slow depending on whether the parameter $G^2$ determined by Eq. (7.12) is small or large when compared to unity. As a collision occurs only when the two-particle levels cross, collisions become more frequent and hence the collision term becomes more important when the scale of collective motion becomes larger. In heavy-ion collisions, the collision term becomes more important as the energy of the colliding system increases because the Pauli principle becomes less inhibitive in preventing the collision between particles. Aside from these general criteria in Table I obtained from our considerations of Eq. (8.8) and the level-crossing formula, there are peculiar cases where the shell effects make the density of single-particle states on top of the Fermi energy irregular. The dependence of the rate of change on the density of single-particle states at the Fermi energy argues for the applicability of the TDHF approximation for closed-shell systems in contrast to the opposite case of the importance of the collision term for open-shell systems. Of course, in such a discussion, the closed-shell nature of the system may change with time and thus the importance of the collision will also undergo changes depending on such a variation.

It is not difficult to envisage that with a large number of particle collisions, a system can attain thermal equilibrium during the course of the dynamical motion, and, subsequently, the quantum stress tensor is characterized not by the totality of the individual nucleonic degrees of freedom, but by a few macroscopic variables such as local density and entropy. The dynamics will then be properly described by nuclear hydrodynamics. Our comparison in Table I indicates that if nuclear hydrodynamics has any region of validity, it is likely to be in large open-shell systems in slow motion with long interaction times. It will be of interest to devise experiments where TDHF approximation and nuclear hydrodynamics can be tested. Recently, an experimental test was proposed[50] to detect the formation of toroids in a head-on or nearly head-on collision of very heavy nuclei such as U on U. The formation of toroids is a hydrodynamical feature[51,52] which appears to be absent in the TDHF dynamics.[10] These toroids, if formed, can be detected by toroidal fission into three or more approximately equal fragments in a nearly coplanar manner (coplanar in the c.m. system).

The equations of motion we have obtained are similar to those in the Fermi-liquid theory.[43] There are notable important differences such as the presence of discrete levels, importance of the mean field, and the absence of a thermal bath. It will be of great interest in future work to explore the implications of the similarities and differences.

With regard to other extensions of the TDHF approximation, the inclusion of pairing (TDHFB) has been discussed previously.[9] Its reformulation in terms of single-particle equations has also been presented.[14] The extension we obtain here in principle includes the pairing interaction but only to the first order. Therefore, it does not include the kind of two-particle correlations of the pairing type. In contrast, the TDHFB approximation includes pairing correlations which, because of the Bogoliubov-Valatin transformation, contains higher-order effects. However, there the collisions between individual nucleons are not included and therefore it cannot be used to discuss the approach to thermal equilibrium and the increase in entropy. What is needed is a unified theory incorporating both pairing and particle collisions. Work is now under way to formulate such a unified theory. Results will be reported later.

With regard to the computational implementation of the ETDHF approximation, the large number of summations one has to carry out in order to evaluate the rate of change of $\partial n_\lambda/\partial t$ in Eq. (6.4) may be a difficult task. Fortunately, the restriction of the $\delta$ function (or a sharp distribution) limits the number of summations. Because much of the important redistribution of occupation probabilities occurs at the Fermi surface, one is well justified in limiting one's attention in this region only, thereby reducing the number of summations. For the residual interaction $v'$, one may use simple $\delta$-function interactions such as the density-dependent Skyrme interaction[53] or those used by Buck and Hill[54] and Marangoni and Saruis.[55] Alternatively, one may even use constant matrix elements as a start. When this is implemented, a calculation with and without particle collisions will illuminate the effect of particle collisions on the dynamics.

Our restriction on the use of only the occupation number but not the occupation number matrix is dictated by practical considerations (see Appendix C). Such an approximation brings with it the unpleasant feature that the result appears to depend on the choice of the representation, as the expectation value of the single-particle Hamiltonian can change drastically by a simple unitary transformation. However, there is in fact not that much arbitrariness in the choice of the basis states. They should be chosen in such a way that the initial occupation matrix is a diagonal matrix, so as to comply with the initial conditions on the degree of occupation of the single-particle states. The

TABLE I. Comparison and contrast of the circumstances in which the TDHF approximation is best applicable to those when the collision term is important.

| TDHF is best applicable | Collision term is important |
|---|---|
| (1) For short interaction time | (1) For long interaction time |
| (2) For small systems[a] | (2) For large systems |
| (3) For rapid motion[b] | (3) For slow motion |
| (4) For small scale collective motion | (4) For large collective motion |
| (5) For closed-shell nuclei | (5) For open-shell nuclei |
| (6) For low energy heavy ion reactions | (6) For moderate energy ($E_{CM} \gtrsim 10$ MeV/$A$) heavy ion reactions |

[a] But sufficiently large so that the mean field can be a good approximation.

[b] But not so rapid as to invalidate the instantaneous effective mean-field approximation.

growth of the off-diagonal occupation matrix elements $n_{\lambda\lambda'}$ occurs near level crossing and depends on the product of the type $\langle\lambda\lambda_3|v'|\lambda_1\lambda_2\rangle\langle\lambda_1\lambda_2|v'|\lambda'\lambda_3\rangle$, where $\lambda$ and $\lambda'$ are different [Eq. (B7)]. As $\lambda$ and $\lambda'$ are not the same, the sum of the products has a tendency to cancel out. One expects that when the number of single-particle states is large enough, the off-diagonal occupation matrix remains approximately diagonal as time proceeds.

The master equation (6.4) we have obtained is physically very transparent and could have been written down directly without recourse to the use of Green's functions. This feature implies that it can also be applied to problems which do not involve a self-consistent mean field. For example, it may be used to study the approach to equilibrium when the mean-field single-particle states are taken to be the Nilsson orbitals, while the collective motion is coupled to the intrinsic degree of freedom through the conservation of total energy. It will be of interest to see how the system approaches thermal equilibrium by following the redistribution of the occupation probabilities when an initially cold nucleus is allowed to oscillate.

In conclusion, we have formulated an extension of the time-dependent Hartree-Fock approximation which includes particle collisions thereby extending the range of validity of the TDHF approximation to regions where irreversible dissipation is important. The formulation opens up a new horizon on the dynamics of many-fermion systems by illuminating the microscopic processes involved in the approach from nonequilibrium to equilibrium.

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## APPENDIX A: TDHF APPROXIMATION IN DENSITY-MATRIX AND SINGLE-PARTICLE FORM

It is well known that starting from the TDHF single-particle equations, the usual TDHF equation in one-body density matrix form can be obtained. Moreover, such a density matrix is idempotent. In the literature, this property and the two forms of the TDHF equation are used interchangeably. However, the proper inverse theorem that the TDHF equation in density matrix form leads uniquely to the TDHF single-particle equations, is, as far as we are aware, never proven explicitly. For this reason, and also for the reason that a thorough understanding of the converse theorem will help the future generalization for cases where the one-body density equation is of a more general form and the density matrix need not be idempotent, we wish to analyze under what explicit conditions the two forms of the TDHF equations are equivalent.

The main arguments in this appendix adopt the following steps. First, we show that under appropriate conditions, a one-body density matrix has the usual bilinear representation in terms of a finite set of orthonormal single-particle wave functions. Then, by construction, we show that, starting with the usual TDHF equation in a density matrix form, the usual TDHF equations in the single-particle form can be uniquely determined.

Given a one-body density matrix $\mathfrak{N}$ which satisfies the following properties:

(i) relation to two-body density matrix $\mathfrak{N}_2$ in the form

$$\mathfrak{N}_2(x_1x_2,x_1'x_2';t)=\mathfrak{N}(x_1,x_1';t)\mathfrak{N}(x_2,x_2';t)-\mathfrak{N}(x_1,x_2';t)\mathfrak{N}(x_2,x_1';t)\,, \tag{A1}$$

(ii) hermiticity:

$$\mathfrak{N}^\dagger(x,x';t)=\mathfrak{N}(x',x;t)\,, \tag{A2}$$

and

(iii) finite normalization:

$$\int dx\,\mathfrak{N}(x,x;t)=N<\infty\,, \tag{A3}$$

then $\mathfrak{N}$ defines uniquely an $N$-dimensional subspace and has a representation

$$\mathfrak{N}(x,x';t)=\sum_{\lambda=1}^{N}\psi_\lambda(x,t)\psi_\lambda^*(x',t)\,, \tag{A4}$$

where $\psi_\lambda$ are orthonormal basis functions which span this subspace.

To prove this, we note that the factorization of the two-body density in the form of one-body density as given by (A1) implies idempotency of the one-body density. This can be readily seen by noting the normalization of $\mathfrak{N}_2$ (Ref. 3),

$$(N-1)\mathfrak{N}(x_1, x_1'; t) = \int dx_2 \mathfrak{N}_2(x_1 x_2, x_1' x_2; t) , \tag{A5}$$

which leads from (A1) to the idempotent property

$$\mathfrak{N}^2 = \mathfrak{N} . \tag{A6}$$

Thus, from conditions (A6) and (A2), $\mathfrak{N}$ has the properties of a projection operator. It follows from standard theorems in operator theory[56] that it decomposes the functional space into two orthogonal subspaces, $S(\mathfrak{N})$ and $S^{\perp}(\mathfrak{N})$, where $S(\mathfrak{N})$ contains eigenvectors of $\mathfrak{N}$ corresponding to the eigenvalue 1 and $S^{\perp}(\mathfrak{N})$ contains eigenvectors corresponding to the eigenvalue 0.

There are then two possibilities to consider. The subspace $S(\mathfrak{N})$ is either finite dimensional or infinite dimensional. For the case of infinite dimensionality, $S(\mathfrak{N})$ is inconsistent with the condition (A3) of finite normalization, and hence must be excluded from further considerations.

Then, for some integer $N$, we have

$$\dim S(\mathfrak{N}) = N . \tag{A7}$$

We then construct a one-body density matrix in terms of an orthonormal basis $\psi_\lambda$ which spans $S(\mathfrak{N})$

$$\tilde{\mathfrak{N}}(x, x'; t) = \sum_{\lambda=1}^{N} \psi_\lambda(xt)\psi_\lambda^*(x't) . \tag{A8}$$

It is easy to show that $\tilde{\mathfrak{N}}$ satisfies conditions (A6), (A2), and (A3). Moreover, operations of $\mathfrak{N}$ and $\tilde{\mathfrak{N}}$ on any arbitrary single-particle wave function lead to the same result, thus implying that $\mathfrak{N}$ and $\tilde{\mathfrak{N}}$ are in fact identical. This completes the proof on the bilinear representation of the idempotent density matrix.

Now, consider the equation of motion for the TDHF density matrix as the starting point:

$$i\hbar\frac{\partial}{\partial t}\mathfrak{N}(x, x'; t) = -\frac{\hbar^2}{2m}(\nabla_x{}^2 - \nabla_{x'}{}^2)\mathfrak{N}(x, x'; t) + \int dx''[v(x, x'') - v(x', x'')][\mathfrak{N}(x, x'; t)\mathfrak{N}(x'', x''; t) - \mathfrak{N}(x, x''; t)\mathfrak{N}(x'', x'; t)] . \tag{A9}$$

An application of the representation (A4) leads to the following:

$$\sum_{\lambda=1}^{N} \psi_\lambda^*(x't)\left(i\hbar\frac{\partial}{\partial t} - h\right)\psi_\lambda(xt) = \sum_{\lambda=1}^{N}\left[\left(i\hbar\frac{\partial}{\partial t} - h\right)\psi_\lambda(x't)\right]^* \psi_\lambda(xt) , \tag{A10}$$

where $\psi_\lambda(x,t)$ are basis functions which span the subspace defined by $\mathfrak{N}$ at time $t$. The single-particle operator $h$ is, in fact, the usual TDHF Hamiltonian, which can be defined by means of the density matrix as follows

$$[h\psi_\lambda](x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi_\lambda(xt) + \int dx'' v(x, x'')\mathfrak{N}(x'', x''; t)\psi_\lambda(xt) - \int dx'' v(x, x'')\mathfrak{N}(x, x''; t)\psi_\lambda(x''t) . \tag{A11}$$

In what follows, it is relevant to note that while the correspondence between $\mathfrak{N}$ and the subspace is unique, so far, the choice of the basis is arbitrary. For example, the basis functions in (A4) under a phase transformation

$$\psi_\lambda(xt) \to \tilde{\psi}_\lambda(xt) = e^{i\theta_\lambda(t)}\psi_\lambda(xt) \tag{A12}$$

leave the density matrix unchanged.

Now, construct the following $N \times N$ time-dependent matrix

$$C_{\lambda\lambda'}(t) = \left\langle \psi_\lambda(t) \left| i\hbar\frac{\partial}{\partial t} - h \right| \psi_{\lambda'}(t) \right\rangle . \tag{A13}$$

Since both $h$ and the subspace $S(\mathfrak{N})$ (and hence the basis functions) vary with time continuously, $C_{\lambda\lambda'}$ is also a continuous function of time. A comparison of both sides of (A10) shows that the matrix $C_{\lambda\lambda'}$ is Hermitian. Moreover, the operator $(i\hbar\partial/\partial t - h)$ leaves the subspace $S(\mathfrak{N})$ invariant. Accordingly, at each time $t$, there exists a diagonalization for the matrix $C_{\lambda\lambda'}$, with real eigenvalues which are also continuous functions of time.

Without loss of generality, we can now take $\psi_\lambda$ to be such a basis which is diagonal with respect to $(i\hbar\partial/\partial t - h)$, so that

$$\left(i\hbar\frac{\partial}{\partial t} - h\right)\psi_\lambda(xt) = \epsilon_\lambda(t)\psi_\lambda(xt) , \tag{A14}$$

where $\epsilon_\lambda(t)$ are the real eigenvalues of the matrix $C_{\lambda\lambda'}$.

We now define the following phase transformation of the single-particle wave functions:

$$\psi_\lambda(xt) \to \tilde{\psi}_\lambda(xt) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \epsilon_\lambda(\tau)d\tau\right)\psi_\lambda(xt) . \tag{A15}$$

It is now easy to show that

$$\left(i\hbar\frac{\partial}{\partial t} - h\right)\tilde{\psi}_\lambda(xt) = 0 , \tag{A16}$$

which is the usual single-particle form of TDHF. This completes our proof of the equivalence of the density matrix and single-particle representations of the TDHF problem.

We note in passing that both Eqs. (A14) and (A16) are equivalent TDHF single-particle equations which follow from the TDHF equation in density matrix form, the difference being an extra purely time-dependent term in the single-particle Hamiltonian which leads to different basis wave functions related by a phase [Eq. (A15)]. The equivalence of these two forms of the single-particle equations has been emphasized recently by Lichtner, Griffin, Schultheis, Schultheis, and Volkov.[16]

## APPENDIX B: MASTER EQUATION FOR OCCUPATION NUMBER MATRIX

We would like to consider a more general representation of the Green's function in the form

$$(-i)g^{<}(1,1') = \sum_{\lambda\lambda'} n_{\lambda\lambda'}\left(\frac{t_1+t_1'}{2}\right)\psi_\lambda(1)\psi_{\lambda}^{*}(1') \tag{B1}$$

with the complementary Green's function

$$ig^{>}(1,1') = \sum_{\lambda\lambda'}\left[1 - n_{\lambda\lambda'}\left(\frac{t_1+t_1'}{2}\right)\right] \times \psi_\lambda(1)\psi_{\lambda}^{*}(1') . \tag{B2}$$

Again, by selecting our basis functions to satisfy the modified TDHF equation (4.4), the equation of motion for the occupation number matrix $n_{\lambda\lambda'}(t)$ is given by

$$\frac{\partial}{\partial t}n_{\lambda\lambda'}(t) = -\frac{1}{\hbar}\int dx_1 dx_1' \psi_{\lambda}^{*}(x_1t)I(x_1t, x_1't) \times \psi_{\lambda'}(x_1't) . \tag{B3}$$

For a slowly varying mean field, we make the same set of simplifying assumptions (5.1) and (5.3) concerning the temporal behavior of the single-particle wave functions. And, instead of Eq. (5.4), we assume

$$n_{\lambda\lambda'}\left(\frac{t_1+t_1'}{2}\right) \simeq n_{\lambda\lambda'}(t_1) . \tag{B4}$$

Then the integration over $E_1$ can be carried out to give

$$\begin{aligned} I(xt, x't^{\dagger}) = -i\int dx''[v'(x,x'') - v'(x',x'')] \\ \times \sum_{\substack{\lambda_1\lambda_2\lambda_3\lambda_4 \\ \lambda_1'\lambda_2'\lambda_3'\lambda_4'}} [(1-n_{\lambda_1\lambda_1'})(1-n_{\lambda_2\lambda_2'})n_{\lambda_3\lambda_3'}n_{\lambda_4\lambda_4'} - n_{\lambda_1\lambda_1'}n_{\lambda_2\lambda_2'}(1-n_{\lambda_3\lambda_3'})(1-n_{\lambda_4\lambda_4'})] \\ \times[\bar{\epsilon}_1 + \bar{\epsilon}_2 - \bar{\epsilon}_3 - \bar{\epsilon}_4 - i\eta]_{\eta\to 0}^{-1}\psi_{\lambda_1}(xt)\psi_{\lambda_2}(x''t)\psi_{\lambda_3'}^{*}(x''t)\psi_{\lambda_4'}^{*}(x_1't)\langle\lambda_1'\lambda_2' - \lambda_2'\lambda_1'|v'|\lambda_4\lambda_3\rangle , \end{aligned} \tag{B5}$$

where

$$\epsilon_i = \tfrac{1}{2}(\epsilon_{\lambda_i} + \epsilon_{\lambda_i'}) . \tag{B6}$$

In consequence, the equation of motion for the occupation matrix is

$$\begin{aligned} \frac{\partial}{\partial t}n_{\lambda\lambda'} = -\frac{1}{\hbar}\sum_{\substack{\lambda_1\lambda_2\lambda_3\lambda_4 \\ \lambda_1'\lambda_2'\lambda_3'\lambda_4'}} [\delta_{\lambda'\lambda_4'}\langle\lambda\lambda_3'|v'|\lambda_1\lambda_2\rangle - \delta_{\lambda\lambda_1}\langle\lambda_4'\lambda_3'|v'|\lambda'\lambda_2\rangle] \\ \times[(1-n_{\lambda_1\lambda_1'})(1-n_{\lambda_2\lambda_2'})n_{\lambda_3\lambda_3'}n_{\lambda_4\lambda_4'} - n_{\lambda_1\lambda_1'}n_{\lambda_2\lambda_2'}(1-n_{\lambda_3\lambda_3'})(1-n_{\lambda_4\lambda_4'})] \\ \times(\bar{\epsilon}_1 + \bar{\epsilon}_2 - \bar{\epsilon}_3 - \bar{\epsilon}_4 - i\eta)_{\eta\to 0}^{-1}\langle\lambda_1'\lambda_2' - \lambda_2'\lambda_1'|v'|\lambda_4\lambda_3\rangle . \end{aligned} \tag{B7}$$

As one can see, an eightfold summation over the complete set of indices of basis functions, which reduces to a sevenfold summation because of the Kronecker δ function, makes the problem intractable in practical calculations.

## APPENDIX C: MASTER EQUATION WITH SPIN AND ISOSPIN AVERAGING

In this appendix, we show how the master Eq. (6.4) can be simplified when the spin and isospin degrees of freedom are averaged over. In particular, we consider the case where the residual interaction depends only on the spatial coordinates,

$$v'(x,x')=v'(|\vec{r}-\vec{r}'|)\,. \tag{C1}$$

We first explicitly introduce the one-particle wave function in the standard product form

$$\psi_\lambda(x,t)=\phi_\alpha(\vec{r},t)\Xi_\sigma(\zeta)\,, \tag{C2}$$

where the single-particle level $\lambda$ represents the collection of the quantum number $\alpha$ labeling spatial wave functions $\phi$ and the quantum number $\sigma$ labeling spin and isospin wavefunctions $\Xi$:

$$\lambda=\{\alpha,\sigma\}\,. \tag{C3}$$

The state $|\lambda_1\lambda_2\rangle$ in Eq. (6.4) is given by the wave function in product form,

$$\psi_{\lambda_1}(\vec{r}_1\zeta_1)\psi_{\lambda_2}(\vec{r}_2\zeta_2)=\phi_{\alpha_1}(\vec{r}_1)\phi_{\alpha_2}(\vec{r}_2)\Xi_{\sigma_1}(\zeta_1)\Xi_{\sigma_2}(\zeta_2)\,, \tag{C4}$$

and the state $|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle$ is given by the antisymmetrized wave function which, for convenience, can be rewritten as a sum of two parts:

$$\psi_{\lambda_4}(\vec{r}_1\xi_1)\psi_{\lambda_3}(\vec{r}_2\xi_2)-\psi_{\lambda_3}(\vec{r}_1\xi_1)\psi_{\lambda_4}(\vec{r}_2\xi_2)=\phi^{(+)}_{\alpha_4\alpha_3}(\vec{r}_1,\vec{r}_2)\Xi^{(-)}_{\sigma_4\sigma_3}(\xi_1,\xi_2)+\phi^{(-)}_{\alpha_4\alpha_3}(\vec{r}_1,\vec{r}_2)\Xi^{(+)}_{\sigma_4\sigma_3}(\xi_1,\xi_2)\,. \tag{C5}$$

In Eq. (C5) the signs (+) and (−) signify the symmetrized and antisymmetrized forms, respectively, with regard to an exchange of the particle coordinates in the wave function in question and $\phi^{(\pm)}$ and $\Xi^{(\pm)}$ are the two-particle spatial and spin and isospin wave functions, respectively:

$$\phi^{(\pm)}_{\alpha_4\alpha_3}(\vec{r}_1,\vec{r}_2)=(1/\sqrt{2})[\phi_{\alpha_4}(\vec{r}_1)\phi_{\alpha_3}(\vec{r}_2)\pm\phi_{\alpha_3}(\vec{r}_1)\phi_{\alpha_4}(\vec{r}_2)] \tag{C6}$$

and

$$\Xi^{(\pm)}_{\sigma_4\sigma_3}(\xi_1,\xi_2)=(1/\sqrt{2})[\Xi_{\sigma_4}(\xi_1)\Xi_{\sigma_3}(\xi_2)\pm\Xi_{\sigma_3}(\xi_1)\Xi_{\sigma_4}(\xi_2)]\,. \tag{C7}$$

From the expressions given in (C4) and (C7), the matrix element of a spatial-dependent residual interaction can now be given in a simple form,

$$\langle\lambda_1\lambda_2|v'|\lambda_4\lambda_3-\lambda_3\lambda_4\rangle=v^{(S)}_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}-\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4})+v^{(A)}_{\alpha_1\alpha_2;\alpha_4\alpha_3}(\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}+\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4})\,, \tag{C8}$$

where the contributions from the symmetric and antisymmetric spatial wave functions are separated and represented by $v^{(S)}$ and $v^{(A)}$, respectively,

$$\begin{Bmatrix} v^{(S)}_{\alpha_1\alpha_2;\alpha_4\alpha_3} \\ v^{(A)}_{\alpha_1\alpha_2;\alpha_4\alpha_3}\end{Bmatrix}=\tfrac{1}{2}\iint d^3r_1d^3r_2\phi^*_{\alpha_1}(\vec{r}_1)\phi^*_{\alpha_2}(\vec{r}_2)v'(\vec{r}_1,\vec{r}_2)\begin{Bmatrix}\phi^{(+)}_{\alpha_4\alpha_3}(\vec{r}_1,\vec{r}_2) \\ \phi^{(-)}_{\alpha_4\alpha_3}(\vec{r}_1,\vec{r}_2)\end{Bmatrix}. \tag{C9}$$

In principle, for each single-particle level $\lambda$, different spatial wave functions can be associated with different spin and isospin components. However, in the case when the spin and isospin degrees of freedom can be averaged over, the resultant master equation is considerably simplified. This is done by considering that, for each set $\lambda$, only the spatial single-particle state $\alpha$ is enough to represent all the spin and isospin substates. The final reduction is achieved by carrying out the summation of the spin and isospin indices in the equation, independent of the spatial wave function indices. This leads to the master equation

$$\begin{aligned}\frac{d}{dt}n_\alpha(t)=\frac{\pi}{\hbar}\sum_{\alpha_2\alpha_3\alpha_4}&\delta(\epsilon_\alpha+\epsilon_{\alpha_2}-\epsilon_{\alpha_3}-\epsilon_{\alpha_4})[(1-n_\alpha)(1-n_{\alpha_2})n_{\alpha_3}n_{\alpha_4}-n_\alpha n_{\alpha_2}(1-n_{\alpha_3})(1-n_{\alpha_4})]\\ &\times(g^{(S)}|v^{(S)}_{\alpha\alpha_2;\alpha_4\alpha_3}|^2+g^{(A)}|v^{(A)}_{\alpha\alpha_2;\alpha_4\alpha_3}|^2)\,,\end{aligned} \tag{C10}$$

where the weighting factors $g^{(A)}$ and $g^{(S)}$ have numerical values of

$$g^{(A)}=6 \tag{C11}$$

and

$$g^{(S)}=10\,. \tag{C12}$$

In passing, we note that, for a zero-range type of residual interaction, there is no contribution from the antisymmetric part of the spatial wave function, and we are left with only the $g^{(S)}$ terms in the master equation.

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