PHYSICAL REVIEW C VOLUME 59, NUMBER 4 APRIL 1999

Self-consistent theory of large amplitude collective motion at finite excitation energy

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(Received 23 July 1998)

We formulate a theory for the transfer of energy from collective degrees of freedom to internal degrees of freedom when the former belong to the adiabatic large-amplitude regime. The framework is that of an extended mean-field theory including dissipation, with the following salient features: (i) The Born-Oppenheimer approximation is extended to finite excitation energy by the introduction of the concept of thermal state, that is pure with respect to collective coordinates and a (square root of *a*) density matrix with respect to internal coordinates. (ii) By assuming that these states form an approximate complete set for application of the Kerman-Klein method, the self-consistent theory of large amplitude collective motion is extended to finite excitation energy. (iii) The mean-field limit is taken, and further study is carried out in the basis of natural orbitals that diagonalizes the one-particle density matrix. In the approximation maintained uniformly in this work, the equations of motion for the orbitals are shown to be of Hamiltonian form; to these are conjoined the master equations for the time rate of change of the occupation numbers. The latter are studied in two extreme limits. In the collisionless limit, dissipation still arises from the response of the mean field to the collective motion (one-body friction). At the opposite extreme, collisions are assumed to be so effective as to force the system always to be in a state of local (constrained) equilibrium. (iv) We review a procedure by which the noncollective variables in the Hamiltonian may be eliminated, leading to equations of motion for the collective variables with dissipative terms that in general depend on the history of the system. The limit of instantaneous friction can be justified in an adiabatic approximation. (v) A decoupling procedure is developed for deriving the form of these equations of motion from the mean-field theory, with the ultimate aim of obtaining the macroscopic parameters that appear in the classical equations of motion for the collective variables. This procedure generalizes that developed in extensive previous work on large amplitude collective motion at zero temperature. (vi) Associating the dissipative equations of motion for the collective variables with one of the assumptions concerning the rates of change of the occupation numbers provides a description of the relaxation of a system initially perturbed from a state of dynamic equilibrium. [S0556-2813(99)05204-8]

PACS number(s): 21.60.Ev, 21.60.Jz, 05.60.−k, 05.70.Ln

I. INTRODUCTION

In the past, writers and their collaborators have developed a self-consistent theory of large amplitude collective motion (LACM) that was based on the assumptions, first, that the degrees of freedom of a many-particle system could be decomposed into two subsets, collective (slow, relevant) and noncollective (fast, irrelevant), and second, that we were at zero temperature, in the sense that excitation energy, if any, remained concentrated in the collective degrees of freedom [1–4]. (Essentially complete references to the work of other authors, as well as to the other work of the authors quoted, will be found in the papers cited.) In this paper we wish to show how the previous theory can be generalized to a situation where the excitation energy is sufficiently high that the exchange of energy between the two subsystems is inevitable. This is a difficult problem with a long history which it would be completely out of place to attempt to review here. Early work may be traced from Ref. [5]. In broad terms, this work dealt with general quantum or semiclassical formulations of transport theory from which one sought to extract an extended one-body approximation that, minimally, included dissipation. More recently, powerful algorithms designed to treat one and two-body correlations on an equal footing have been formulated and applied, using either a density matrix, i.e., one-time formalism [6–8] or a real-time Green's function approach [9–11]. This work, however, is not yet capable of dealing with problems of large amplitude collective motion.

In this paper, we shall make no effort to provide yet another general version of transport theory. Rather, we are interested in developing the formalism for the case that the exchange of energy between the collective and noncollective degrees of freedom can be described in a Born-Oppenheimer (BO) approximation. The work that follows is most closely connected in aim with a previous paper involving one of us [12], but differs markedly from that work in concept and in execution. Selected papers that bear some relation to the subject of self-consistent LACM at finite excitation energy are [13–18]. It is also appropriate to mention several microscopic approaches, not fully self-consistent in our sense, but extensively worked out and with a track record of successful applications. We refer to the linear response method of Hoffman and associates [19] and dissipative diabatic dynamics due to Nörenberg and collaborators [20,21]. It would be particularly interesting to try to incorporate some of the latter ideas into our work, but this will not be attempted here.

The way in which the extension of the BO approximation to finite excitation energy is carried out is described in Sec. II. There we introduce the idea of thermal state, which need not be a state of thermal equilibrium, but naturally includes the latter as a subclass. Application of this concept within the framework of the Kerman-Klein method [22,23], in Sec. III, followed by a passage to a semiclassical approximation, leads to the general dynamical equations that underlie the remainder of the development. Not surprisingly we come down to a mean-field description extended to include two-particle collisions. In this work, however, we confine our efforts to an approximation in which the basic element remains the one-particle density matrix. In Sec. IV, we study this object in the basis of natural orbitals, namely, the representation in which it is diagonal, and identify the independent dynamical elements of the problem. We also describe the special limits that allow us to deal simply with the problem of collisions.

The endgame of our exercise is to derive classical ''macroscopic'' equations describing the thermalization of a system initially excited into collective motion. Thus we must specify a set of classical equations that is consistent in form with the microscopic structure of the theory as well as provide a method for the determination of the parameters that occur in these equations. The former discussion is carried out in Sec. V, where the central issue addressed is the derivation of the equations of motion for the collective submanifold including dissipation, starting from a classical Hamiltonian for the total system. The microscopic basis for the starting equations of Sec. V is given in Sec. VI, which contains an outline of the calculations that actually have to be done to implement the theory. The procedure put forth generalizes the previously developed self-consistent theory of LACM, valid for zero temperature. Section VII contains a summary of our work that highlights the essential steps in the derivation of the final transport equations, reviews briefly how to utilize the resulting equations, and suggests further extensions of the formalism.

Further discussion of thermal states can be found in Appendix A. In Appendix B, we describe another argument that generalizes the Kerman-Klein method to finite temperature, applicable as given only to the case of thermal equilibrium, and in Appendix C, we record a few details concerning some of the results of Sec. VI.

Before beginning the detailed exposition, it may be helpful to augment the preceding brief statement of the contents of this paper by providing an account of how we reached the shape and content of the material that follows. The original impetus was to try to simplify the self-consistent theory of nonequilibrium processes developed in Ref. [12]. There the variables used to describe a system were pairs of canonical variables, equivalent to the ones that will be introduced in this work in Sec. II by applying a Wigner transform to a quantum transition amplitude; in addition one encounters a set of occupation numbers of single-particle states. Just as at zero temperature, the problem is simplified by focusing on at most a few canonical pairs approximately decoupled from the remaining space, but there was no apparent way of selecting a subset of the occupation numbers, and this rendered the formalism too complicated to apply. Our original goal was to construct a formalism in which we would replace all the occupation numbers by temperature or entropy.

Though this aim is achievable only in special cases, as we shall learn, it served the purpose of leading us to the concept of thermal state, introduced in Sec. II, followed in Sec. III by its application to the (quantum) equations of motion, thus providing us with a basis for a quantum theory of transport. In this paper, however, this theory is utilized only as a convenient way of passing to a classical description for the dynamical variables. The first (familiar) climax of these considerations is Eq. (3.4), which is the standard mean-field equation for the one-particle density matrix plus (so-far unspecified) corrections that describe dynamical correlations.

The next step in understanding how to deal with this equation was to study, in Sec. IV, the Hermitian one-particle density matrix in its diagonal form, namely in the basis of natural orbitals, Eq. (4.1). Though the matrix itself is diagonal, its time derivative is not. We first considered the off-diagonal equations of motions. It is well known (see [13] and references therein) that off-diagonal correlation terms are the source of dissipation of the mean-field energy due to two-particle interactions. By choosing to drop this term, we find that the remaining equations have the structure of Hamilton's classical equations of motion. This allows us to apply the theory of canonical transformations in order to introduce a representation in which the variables separate into collective and noncollective sets, using the machinery described in [3]. The details of this procedure are, however, postponed until Sec. VI.

The question that one may legitimately ask at this point is whether we would be stymied if we were to reinstate some approximation to the discarded two-body dissipation, because if this were the case, the value of the current work would be seriously compromised. Our answer is that we could still carry out a transformation, leading to a modified form of the Hamiltonian equations of motion (5.4)–(5.7), of which the first two sets refer to the collective variables and the last two to the non-collective variables. In these equations there is naturally no overt sign of dissipation. The burden of Sec. V is to show how friction arises when the noncollective variables are eliminated from these equations, leading to a conventional Newton's equation with friction, Eq. (5.41), for the collective variables. (This is the so-called one-body friction having its origin in a ''time-dependent'' mean-field.) If we were to retain the two-body friction term, Eqs. (5.4)–(5.7) would at this stage contain explicit dissipative terms, which would be part of the final result.

The results of this paper can be used to study the following problem: Given a set of initial conditions specified by the collective coordinates and velocities and by a set of occupation numbers, which are the diagonal elements of the density matrix, how does the system relax to equilibrium? The dissipative motion can be studied with the help of the Newton equation of motion (5.41). In this equation the quantities that enter, the mass matrix, the conservative forces, and the friction tensor are all functions not only of the instantaneous values of the collective coordinates, but also of the set of occupation numbers. The equations of motion for the latter, the so-called master equations are the content of the diagonal elements of the equations of motion.

This brings us to what still remains the most serious practical difficulty facing a self-consistent theory of transport such as formulated in this paper. The elements in the final Newton equation are to be calculated by the method described in Sec. VI. This requires the solution of a nonlinear problem, the so-called local harmonic approximation, over a multidimensional manifold which is the direct product of the Lagrangian manifolds associated with the collective coordinates and the multidimensional space of the occupation numbers. We consider only two tractable limits for the treatment of the occupation number space. The first is the natural preserve of the mean-field approximation in which the occupation numbers are fixed as we move away from thermal equilibrium; in this case the entire manifold of occupation numbers is replaced by the entropy variable, and there is no necessity to adjoin a master equation to the Newton equation. In the other limit, in which we assume that the system is always in a configuration of (constrained) local equilibrium, as we explain in the text, the space of occupation numbers can be replaced by the temperature as the single variable. The slow change of the temperature with time, as given by Eq. (4.18), is derived from an equation which is a linear combination of all the master equations, determined by an approximate condition of conservation of mean-field energy and the local Fermi distributions. In any event, both in the general case and in the special cases, we end up with a theory that is classical in the treatment of the collective variables and quantum in the treatment of the occupation numbers.

II. CONCEPT OF THERMAL STATES

In our applications, we shall have in mind the nuclear many-body problem, described by a general shell-model Hamiltonian of the form

$$\hat{H}=h_{\alpha\beta}a^{\dagger}_{\alpha}a_{\beta}+\frac{1}{4}V_{\alpha\beta\gamma\delta}a^{\dagger}_{\alpha}a^{\dagger}_{\beta}a_{\delta}a_{\gamma}. \tag{2.1}$$

The single-particle basis designated by the first few letters of the Greek alphabet refer to an arbitrary choice of such a single-particle set. The formalism developed below will also apply to the more general case of a given energy functional of any order in density, kinetic-energy density, etc., without changes in the essence of the construction. The assumption (2.1) just simplifies the further considerations.

We begin with a discussion of the basis of states for the many-body system that will be utilized in the following developments, leading below to the concept of thermal state. We assume that we can introduce a localized basis:

$$|Q,q\rangle=|Q)|q], \tag{2.2}$$

where Q refers to the collective coordinates and q to the noncollective coordinates. Note the use of the angular bracket, parenthesis, and square bracket to distinguish total space, collective space, and noncollective space, respectively. We shall adopt a generalized BO picture of the eigenstates of the Hamiltonian, designating them as $|n,f\rangle$. For low excitation energies, we may assume that n represents quantum numbers of a collective band and that f is an ordering number for these bands that is associated with the state of excitation of the fast (noncollective) system. For higher excitation energies, we shall continue to use the same designation, but its physical meaning is perhaps less clear, except when a simple spectrum (such as a set of harmonic oscillators) may be associated with the noncollective spectrum. We represent the states $|n,f\rangle$ in the form

$$|n,f\rangle=\sum_{f'}\int dQ|Q,f'\rangle\langle Q,f'|n,f\rangle, \tag{2.3}$$

$$|Q,f\rangle=|Q)|f{:}Q]\equiv|Q)|f], \tag{2.4}$$

$$|f{:}Q]=\int dq|q][q|f{:}Q]. \tag{2.5}$$

The expanded notation, $|f{:}Q]$, which we now suppress, is meant to indicate that the states of the fast system adjust to the instantaneous position Q of the slow system, which is the basic adiabatic assumption. We have

$$\langle Q,f|Q',f'\rangle=\delta(Q-Q')\delta_{ff'}. \tag{2.6}$$

Let us, for the moment, focus on the basis vectors (2.4). At $T=0$ we can associate with it a pure-state N-body density

$$\hat{D}=|Q)|f][f|(Q|. \tag{2.7}$$

(This is to be contrasted with the density $|nf\rangle\langle fn|$ that we would actually use to calculate physical averages.) At finite excitation energy, this is replaced by an incoherent average in the intrinsic space yielding a mixed state

$$\hat{D}=|Q)\underbrace{\sum_{ff'}|f]d_{ff'}[f'|}_{\hat{d}}(Q|, \tag{2.8}$$

where the density in the intrinsic subspace has been abbreviated as $\hat{d}$. This is some arbitrary density at the moment. Below it will be specialized to a density valid for the characterization of the BO approximation.

Our motivation for introducing the construct (2.8) is by no means obvious. It is not meant to be directly useful in the standard sense of averaging with operators to provide expectation values of physical observables. Instead it is recorded as a (possibly helpful) intermediate step motivating the introduction of its square root, the thermal state, Eq. (2.9). With the latter we aim at providing a mixed description that is, nevertheless, coherent with respect to the collective dynamics. By coherent we mean that we can (and shall) calculate matrix elements of operators between thermal states with different Q, these states sharing, in this respect, the property of a pure state. Because of this property, the thermal state was first visualized as a ''natural'' tool for a generalization of the BO approach to finite excitation energy within the framework of the equations of motion method, as described in Sec. III. Based on our previous experience, there was the further expectation that it would provide an appropriate means for reaching the mean-field approximation.

Note that the development below depends for its validity only on the form of Eq. (2.8). A further specialization is to a density $\hat{d}(Q,T)$, describing a system to which a temperature can be assigned at all times, even if the system is not in overall equilibrium. We refer to this case as local or constrained equilibrium. This will be one of the special cases treated in this paper.

We now introduce a construct that can be thought of as providing some quantum-mechanical underpinning for our ultimately classical considerations. We break the bilinear full density (2.8) back again into co- and contravariant linear pieces yielding a ''thermal state''

$$|Q,d\rangle=|Q)\hat{d}^{1/2}, \tag{2.9}$$

where $\hat{d}^{1/2}$ can be any square-root of the intrinsic density $\hat{d}$. For simplicity, we use here the Hermitian square root. We can also write this state in the form

$$|Q,d\rangle=|Q)\sum_{ff'}|f]a_{ff'}[f'|, \tag{2.10}$$

and see that the coefficients $a_{ff'}$ therein are just the elements of $\hat{d}^{1/2}$. They fulfill the conditions

$$\sum_{\tilde{f}} a_{f\tilde{f}}a^{*}_{f'\tilde{f}}=d_{ff'}\,. \tag{2.11}$$

The state (2.9) has the property, essential for our needs, that its dual product reproduces the full density (2.8), i.e.,

$$\hat{D}=|Q,d\rangle\langle Q,d|=|Q)\hat{d}(Q|, \tag{2.12}$$

and with it all expectation values, products, etc.

It is important to emphasize once more that the considerations to this point (and for the rest of this paper) also apply to systems more general than thermal equilibrium. Some further discussion and especially comparison with the concepts of thermal-field theory will be found in Appendix A. In the next section, we show how the description introduced in this section can be incorporated into the dynamical description of our nuclear system. The net result is Eq. (3.4) below for the time dependence of the single-particle density matrix, which is generated both by a mean field and by a ''collision'' term.

Thus far the state $\hat{D}$ as given in Eq. (2.12) represents one localized point of a collective manifold. Our ultimate aim is the description of collective dynamics which connects various points of the manifold. Consequently, one has to deal with nondiagonal matrix elements $\langle Q,d|\hat{A}|Q',d'\rangle$. It is customary to express this in the spirit of a semiclassical picture through coordinate Q and momentum P. Toward that end, we follow the well-worn path of introducing the Wigner transform. Suppressing for the instant the intrinsic structure, we therefore compute

$$A(\overline{Q},P)=\int d\tilde{Q}\,\exp(-iP\tilde{Q})\langle Q|\hat{A}|Q'\rangle, \tag{2.13}$$

$$\tilde{Q}=Q-Q', \tag{2.14}$$

$$\overline{Q}=\frac{1}{2}(Q+Q'). \tag{2.15}$$

Provided that the ingredient matrix elements of $\hat{A}$ and $\hat{B}$ are strongly peaked in $\tilde{Q}$ and slowly varying in $\overline{Q}$, we then have for the classical limit of a product,

$$\begin{aligned} C(\overline{Q},P)&=\int d\tilde{Q}dQ''\exp(-iP\tilde{Q})\langle Q|\hat{A}|Q''\rangle\langle Q''|\hat{B}|Q'\rangle\\ &\cong A(\overline{Q},P)B(\overline{Q},P), \end{aligned} \tag{2.16}$$

i.e., the Wigner transform of a matrix product is approximately the product of the individual Wigner transforms.

There remains the question of how to characterize the degrees of freedom buried in the intrinsic state $\hat{d}$. In the zero temperature (fully coherent) limit, this state is characterized by a set of non-collective coordinates q, usually treated in practice in the small vibration limit. In the classical limit these become the conjugate pairs (q,p). The theory to be developed suggests that also at finite temperature one can extract a coherent set of noncollective variables. There remains, however, an additional incoherent structure, currently assigned an identification label ν, to be identified later as a set of occupation numbers. Thus we rewrite the thermal states as

$$|Q,d\rangle\equiv|Q,q,\nu\rangle. \tag{2.17}$$

These are still mixed states in the sense that we cannot form linear combinations of them. It is furthermore assumed that for transition matrix elements between different thermal states, the value of ν is fixed, whereas q shares the same behavior as Q. Finally this means that for the full physics the quantity (2.13) is replaced by the quantity $A(\overline{Q},P,\overline{q},p,\nu)$. In the sequel, we drop the bars. The way in which these constructs play their role will be seen in the next section.

III. BASIC DYNAMICAL EQUATIONS

We study the dynamics of the system starting with the equation of motion for the ''particle-hole'' operator

$$\hat{\rho}_{\alpha\beta}=a^{\dagger}_{\beta}a_{\alpha}, \tag{3.1}$$

namely

$$\begin{aligned} i\frac{d}{dt}\hat{\rho}_{\alpha\beta}=[\hat{\rho}_{\alpha\beta},\hat{H}]=h_{\alpha\gamma}\hat{\rho}_{\gamma\beta}-\hat{\rho}_{\alpha\gamma}h_{\gamma\beta}\\ +\frac{1}{2}V_{\alpha\gamma\delta\epsilon}a^{\dagger}_{\beta}a^{\dagger}_{\gamma}a_{\epsilon}a_{\delta}\\ -\frac{1}{2}V_{\delta\epsilon\beta\gamma}a^{\dagger}_{\delta}a^{\dagger}_{\epsilon}a_{\gamma}a_{\alpha}. \end{aligned} \tag{3.2}$$

At the next stage we take the matrix element of this equation between two different thermal states (with the same value of ν, see above). To evaluate matrix elements of two body operators, we introduce a generalized factorization (letting Q stand for Q,q,ν),

$$
\begin{aligned}
\langle Q|a_\beta^\dagger a_\gamma^\dagger a_\epsilon a_\delta|Q'\rangle &\equiv \rho^{(2)}(\delta\epsilon Q'|\gamma\beta Q) \\
&= \frac{1}{2}\{\langle Q|a_\gamma^\dagger a_\epsilon|Q''\rangle\langle Q''|a_\beta^\dagger a_\delta|Q'\rangle \\
&\quad -(\epsilon\leftrightarrow\delta)-(\beta\leftrightarrow\gamma)+(\epsilon\leftrightarrow\delta,\beta\leftrightarrow\gamma)\} \\
&\quad +c^{(2)}(\delta\epsilon Q'|\gamma\beta Q). \qquad (3.3)
\end{aligned}
$$

This equation should first of all be viewed as a definition of $c^{(2)}$, the correlated part of the two-body density matrix. In all past applications, we have simply dropped this term, so that the resulting equation becomes an approximation, the generalized density matrix or ‘‘Kerman-Klein’’ approximation. For the class of problems under study, we shall eventually have to go beyond these previous treatments, though in this paper, we shall make simplifying assumptions that will allow us to postpone the problem of including $c^{(2)}$.

Taking the Wigner transform of Eq. (3.3) and applying the convolution theorem for a product in the approximate form (2.16), we obtain the equations that are fundamental to our further studies,

$$
i\frac{d}{dt}\rho_{\alpha\beta}=[\mathcal{H},\rho]_{\alpha\beta}+\mathcal{I}_{\alpha\beta}. \qquad (3.4)
$$

Here $\mathcal{H}$ is the mean field Hamiltonian

$$
\mathcal{H}_{\alpha\beta}(Q,P,q,p,\nu)=h_{\alpha\beta}+\mathcal{V}_{\alpha\beta}(Q,P,q,p,\nu), \qquad (3.5)
$$

$$
\mathcal{V}_{\alpha\beta}(Q,P,q,p,\nu)=V_{\alpha\gamma\beta\delta}\rho_{\delta\gamma}(Q,P,q,p,\nu). \qquad (3.6)
$$

The last term in Eq. (3.4), often designated simply as the collision term, represents, in fact, all the physics consequent upon the inclusion of the two-particle correlation function $c^{(2)}$, and thus not included in the mean field approximation. In this sense Eq. (3.4) is still exact.

We have already alluded [6–11] to the theoretical and practical advances that have been made in the study of the problem of the collision term. Our purposes are best served by reference to the treatment by Ayik [13]. He shows that in a weak-coupling approximation the diagonal part of the collision term (in the basis of natural orbitals discussed below) is the well-known collision term in the Boltzmann-Uhlenbeck (BU) equation, whereas the off-diagonal part provides the explicit two-body friction term in the equations of motion (as well as a change of the self-consistent field in the general non-Markovian situation).

In the development that follows, we have chosen to neglect the off-diagonal collision term. This means that the remaining theory can only describe one-body friction. The retention of the BU term leads nevertheless to a well-defined problem, which we treat only in several limiting cases.

It is only in consequence of the neglect of two-body dissipation that we shall be able to directly generalize our zero-temperature version of LACM to finite excitation energy. A further extension to include the off-diagonal terms appears to be feasible and will be the subject of a future investigation.

IV. DENSITY MATRIX IN THE BASIS OF NATURAL ORBITALS

Equation (3.4) is the basic dynamical equation from which we want to extract the description of the collective motion in terms of the density matrix, $\rho(Q,P,q,p,\nu)$, that defines the collective manifold. We shall divide this procedure into several distinct steps. In the first step, carried out in this section, we introduce the description of the density matrix in terms of natural orbitals and thus identify the elements that are singled out for further study. The equations satisfied by these elements are determined by the application of Eq. (3.4). We study what can be learned from this equation without specifying in detail the classical dynamics of the collective coordinates.

Already at this stage, it is possible to specify the shape and content of the most general problem we can hope to study with the formalism of this paper, which is a mixed classical-quantum transport or relaxation problem. The formulation to be presented in this section will, however, be too complex to be dealt with practically. It will be too complex for two reasons. The first is that though we shall identify a classical Hamiltonian system as a subsystem of the extended mean-field theory, it has far too many degrees of freedom (even an infinite number) for us to consider realistically. Thus, an essential element of the development will require us to seek a canonical transformation to a phase space in which we can separate off one or a few collective degrees of freedom from the full symplectic manifold. The second reason is that we are also not equipped to treat in full generality the quantum part of the problem, that will describe the time rates of change of occupation numbers brought about by collisions.

The problem of studying the Hamiltonian system will take up most of the remainder of this paper. Orientation for the study of this problem will be provided beginning in the next section.

Turning then to the first part of our task, we introduce the diagonal or natural orbital version of the one-body density matrix,

$$
\rho=\sum_a n_a|\varphi_a)(\varphi_a|, \qquad (4.1)
$$

where the $|\varphi_a)$ are a complete set of orthonormal functions and the n_a are correspondingly the occupation numbers for those orbits. As a consequence, we shall show in this section that the equations of motion can be decomposed into two subsets. The first, which describes the time rate of change of the single-particle basis, will be seen to have the form of Hamilton’s classical equations of motion, generalizing the previous considerations at zero temperature. The second set, often called master equations, describes the rate of change of the occupation numbers brought about by collisions.

To obtain equations for the elements contained in the form (4.1), namely, the single-particle wave functions and the occupation numbers, we study this form in conjunction with the equation of motion (3.4). For instance, we would like to find the equation satisfied by the single-particle functions $|\varphi_a)$. Toward this end, it is convenient to consider an infinitesimal change in ρ. To conserve the norm of the single-particle functions, we have

$$\delta|\varphi_a)=\sum_{b\neq a}|\varphi_b)\delta r_{ba}, \quad \delta r^*_{ba}=-\delta r_{ab}. \tag{4.2}$$

As a consequence, we can write

$$\delta\rho=\sum_{b>a}|\varphi_b)\delta r_{ba}(n_a-n_b)(\varphi_a|+\sum_{b>a}|\varphi_a)$$
$$\times\delta r^*_{ba}(n_a-n_b)(\varphi_b|+\sum_a|\varphi_a)\delta n_a(\varphi_a|, \tag{4.3}$$

an expression that clearly separates off-diagonal and diagonal contributions.

Let us first consider the off-diagonal pieces in an approximation in which we ignore the off-diagonal elements of the collision term. This approximation underlies our subsequent treatment of the off-diagonal elements of the equations of motion and is an essential simplification. From Eqs. (3.4) and (4.3) we can therefore write (together with the complex conjugate relation)

$$i\frac{d}{dt}r_{ba}=\mathcal{H}_{ba}, \quad b>a, \tag{4.4}$$

and furthermore, with W equal to the instantaneous Hartree-Fock energy,

$$W=\mathrm{Tr}\,h\rho+\frac{1}{2}\mathrm{Tr}\,\mathrm{Tr}\,\rho V\rho \tag{4.5}$$

we have

$$\mathcal{H}_{ba}=\frac{\delta W}{\delta\rho_{ab}}=\frac{\delta W}{\delta r_{ab}}\frac{1}{(n_b-n_a)}. \tag{4.6}$$

If we understand that the eigenvalues n_a have been arranged in descending order and that henceforth we follow the convention $b>a$ (and therefore $n_a>n_b$), it follows that Eq. (4.4) can be rewritten

$$i\frac{ds_{ba}}{dt}=\frac{\delta W}{\delta s^*_{ba}},$$

$$\delta s_{ba}=\sqrt{n_a-n_b}\,\delta r_{ba}. \tag{4.7}$$

These equations and their complex conjugates demonstrate that the off-diagonal elements of the equations of motion are of the form of Hamilton's canonical equations of motion for the complex canonical coordinates s_{ba} and is^*_{ba}.

Though this result is to some extent similar to what we have found previously at zero temperature, there are two essential differences. The first is that the number of degrees of freedom of the equivalent dynamical system is much larger than at zero temperature, comprising particle-particle and hole-hole pairs in addition to particle-hole pairs. The second is that, as just shown, the Hartree-Fock energy serves as Hamiltonian only at fixed occupation number. It is now apparent that it is the occupation numbers that constitute the elements of the set ν, hitherto unspecified, on which the density matrix elements depend.

It remains for us to specify the dynamics of the occupation numbers. According to Eqs. (3.4) and (4.1), we have the equation

$$i\frac{dn_a}{dt}=\mathcal{I}_a(\mathbf{n},\mathbf{s}), \tag{4.8}$$

wherein the right-hand side, the ''collision term'' is specified as a function of the sets $\mathbf{n}=\{n_a\}$, $\mathbf{s}=\{s_{ba}\}$. Together with Eq. (4.7) we have arrived at the following formulation: Mean field theory with collisions is equivalent to two sets of equations for the elements of the one-particle density matrix in the basis of natural orbitals. One set, Eq. (4.7), describes the rates of change of the orbitals and is of Hamiltonian form. The second, Eq. (4.8), is for the rates of change of the occupation numbers. Together these independent elements define an initial value problem which describes the relaxation of a system of fermions initially perturbed away from equilibrium.

Most of the considerations that begin in the next section are concerned with making further approximation in these equations, in particular the Hamiltonian set, in order to bring them into a more useful form. None of these manipulations, however, will change the fundamentals as we have just outlined them. For the remainder of this section, we review and develop some important and useful properties of the formalism.

In Sec. VI, we shall study transformations from the set **s** (or **r**) to the preferred canonical set (Q,P,q,p). Imagine for the moment that this has been done. For fixed occupation numbers, we thus can consider $r=r(Q,P,q,p)$. Consequently we can write Eq. (4.4) in a more explicit form by using

$$\frac{dr_{ba}}{dt}=[\dot{Q}\partial_Q+\dot{P}\partial_P+\dot{q}\partial_q+\dot{p}\partial_p]r_{ba}\equiv\dot{z}\partial_z r_{ba}. \tag{4.9}$$

This explicit form allows us to display the single particle equations that determine the functions φ. The most general form consistent with Eqs. (4.4) and (4.9), from which the former may be derived, is

$$[\epsilon_a-\mu+i\dot{z}\partial_z]|\varphi_a)=\mathcal{H}|\varphi_a). \tag{4.10}$$

This has the form of a constrained Hartree-Fock equation with eigenvalue ϵ_a, and μ is the chemical potential. Equation (4.10) can be derived from the variational principle

$$\delta\left[\mathcal{W}-\sum_a\epsilon_a n_a(\varphi_a|\varphi_a)\right]=0, \tag{4.11}$$

where

$$\mathcal{W}\equiv W-\sum_a(\varphi_a|n_a[-\mu+i\dot{z}\partial_z]|\varphi_a) \tag{4.12}$$

is the constrained mean field energy, W is the mean-field energy defined in Eq. (4.5), and the variations are carried out with respect to the single-particle functions.

For the special case of instantaneous local equilibrium of the single-particle degrees of freedom, the previous considerations may be supplemented by the requirement that we maximize the mean-field entropy

$$S=-\sum_a n_a \ln(n_a)-\sum_a (1-n_a)\ln(1-n_a), \quad (4.13)$$

with respect to the choice of the occupation numbers n_a, subject to a fixed value for the constrained mean-field energy $\mathcal{W}$. This yields after a standard manipulation the expected result

$$n_a=\{1+\exp[\beta(\epsilon_a-\mu)]\}^{-1},$$

$$\epsilon_a=(\varphi_a|\mathcal{H}|\varphi_a). \quad (4.14)$$

We consider finally the question of conservation of the mean-field energy. Using the equations of motion (4.7), we find easily

$$\frac{dW}{dt}=\sum_a \epsilon_a \frac{dn_a}{dt}, \quad (4.15)$$

$$\epsilon_a=h_a+\sum_b V_{abab}n_b. \quad (4.16)$$

Obviously W is conserved if we ignore collisions ($dn_a/dt=0$). This will be one of the limits that we consider.

On the other hand, it has been shown [13] that the right-hand side of Eq. (4.15) vanishes approximately even in the presence of collisions. This follows if one substitutes for $\dot{n}_a$ the usual form of collision term, namely the Boltzmann form with Pauli corrections (the Boltzmann-Uhlenbeck form) in the approximation in which the sum of the single particle energies is conserved. Thus the total mean-field energy continues to be conserved even in the presence of collisions, which are responsible, nevertheless, for the exchange of energy between the collective and non-collective degrees of freedom.

It is a further stretch to assume that we can apply conservation of mean-field energy even in the strong-collision limit, which we define as one in which, in a relaxation process, the system passes only through states of local equilibrium. This requires, in general, that the equilibration time be short compared to the period of the collective motion. In general, we may expect this limit to be valid, if at all, only at high energies of excitation, whereas we know that the no-collision limit is valid at low excitation, where collisions are suppressed by the Pauli principle.

The strong collision limit can be treated almost as simply as the no collision limit. As will be clear from the discussion to be given in Sec. VI, in this case the dynamic-thermal collective manifold is specified by values of Q and β, and the combinations

$$\mathcal{E}_a(Q,\beta)\equiv\epsilon_a-\mu \quad (4.17)$$

will be determined as functions of these variables alone. This is a tremendous simplification compared to the general case, where, as we shall see, the collective manifold is specified by Q and the full set of occupation numbers.

Under these conditions, as we now compute, the conservation-of-energy condition will determine a relationship between $\dot{\beta}$ and $\dot{Q}$ that will serve as one of the driving equations for the description of the relaxation process. Thus, from the vanishing of the right-hand side of Eq. (4.15), by substituting Eq. (4.14), at the same time taking Eq. (4.17) into account, we obtain

$$\dot{\beta}=-\frac{\sum_a \beta\mathcal{E}_a \dfrac{\partial\mathcal{E}_a}{\partial Q}\dfrac{\exp(\beta\mathcal{E}_a)}{[1+\exp(\beta\mathcal{E}_a)]^2}}{\sum_a \left[\mathcal{E}_a^2+\beta\mathcal{E}_a\dfrac{\partial\mathcal{E}_a}{\partial\beta}\right]\dfrac{\exp(\beta\mathcal{E}_a)}{[1+\exp(\beta\mathcal{E}_a)]^2}}\dot{Q}. \quad (4.18)$$

In the strong collision limit, as we have defined it, this equation replaces the entire panoply of rate equations for the occupation numbers.

V. CLASSICAL EQUATIONS OF MOTION WITH DISSIPATION

A logical next step in the development might be the derivation of the canonical transformation to collective and intrinsic coordinates that provides optimum decoupling of the collective pairs (Q,P) from the noncollective pairs (q,p). We postpone these considerations to the next section. In this section, we shall suppose once more that this step has been carried out. We then use the resulting equations of motion to ''eliminate'' the noncollective degrees of freedom from the equations of motion leading to equations of motion for the collective coordinates that contain explicit dissipative terms. This is by far the longest argument given in detail in this paper, leading to Eq. (5.40), even more familiar in the form (5.41).

We thus turn to a derivation of the equations for a dissipative collective dynamics from''first principles.'' This is also a subject with a long history. For a recent review with extensive bibliography, see [24]. We shall not attempt to do any justice to this topic, but simply present the material in the form that we require it.

We suppose the full many-particle system, with all degrees of freedom included, to be described classically by the Hamiltonian

$$H=V(Q,q,p)+\frac{1}{2}B^{ij}(Q,q,p)P_iP_j+A^i(Q,q,p)P_i. \quad (5.1)$$

Here, the lower case q and p refer to the noncollective variables that run over a set of indices labeled by a (not to be confused with the like index on the single-particle functions). So far, we have expanded only in powers of the collective momenta. The choice of variables in Eq. (5.1) can be considered to result from a canonical transformation at fixed occupation numbers from the variables s_{ba}, is^*_{ba} that have been identified previously as canonical. Thus Eq. (5.1) can be viewed (to the second order in P) as formally equivalent to the original mean-field Hamiltonian W for a fixed set of occupation numbers. Further details concerning the conditions that determine the mapping

$$s_\alpha = s_\alpha(Q,P,q,p) \tag{5.2}$$

are discussed in the next section.

In order to be able to present our arguments as explicitly as possible, we specialize the form (5.1) to the small amplitude approximation in the intrinsic space. In this approximation it becomes

$$H = V(Q) + \frac{1}{2}B^{ij}(Q)P_iP_j + \frac{1}{2}V_{ab}(Q)q^aq^b + \frac{1}{2}B^{ab}(Q)p_ap_b + V_a(Q)q^a + B^{ai}(Q)p_aP_i. \tag{5.3}$$

Here V_a and V_{ab} are first and second partial derivatives of V evaluated at $q=0$. The problem of determining the potential and mass coefficients that occur in this expression is precisely the problem of determining the canonical transformation from the original form of the mean field Hamiltonian.

In the equations of motion that follow and any further manipulation of them we shall consistently and without additional disclaimers limit ourselves to terms of the first order in q and p. From Eq. (5.3) we thus have

$$\dot{Q}^i = B^{ij}P_j + B^{ia}p_a, \tag{5.4}$$

$$\dot{P}_i = -V_i - V_{ia}q^a, \tag{5.5}$$

$$\dot{q}^a = B^{ai}P_i + B^{ab}p_b, \tag{5.6}$$

$$\dot{p}_a = -V_a - V_{ab}q^b. \tag{5.7}$$

Without further loss of generality, we introduce normal coordinates in the intrinsic space. This allows us to replace the quantities B^{ab} by unity and the quantities V_{ab} by ω_a^2 and suppose that all remaining force and mass coefficients refer to the new coordinates. The distinction between covariant and contravariant indices now becomes irrelevant in the intrinsic space. Henceforth all such indices will be written as subscripts.

We cannot emphasize too strongly that to the approximations considered (convenient for the explicit derivations carried out below), Eqs. (5.4)–(5.7) are completely equivalent to Eq. (4.7). Here the macroscopic parameters B^{ij}, etc., are functions

$$B^{ij} = B^{ij}(Q, n_a). \tag{5.8}$$

The canonical transformation that leads to Eq. (5.1) is carried out at fixed n_a, i.e., there are infinitely many such canonical transformations, one for each set of n_a. Furthermore, in principle, we can at this point study the initial value or relaxation problem by adjoining the master equations (4.8) to (5.4)–(5.7).

For a system with a finite number of degrees of freedom, this might well be a practical and straightforward calculation. An application of interest would be to consider a set of initial conditions in which all the energy was concentrated in the collective degrees of freedom. We would then ask how, in the course of time this energy is transferred to the other degrees of freedom. For a small number of coordinates overall, we would expect energy to reconcentrate from time to time in the collective coordinates. As the number of noncollective coordinates increases, we expect this recurrence time to increase. Beyond some point it becomes more sensible to talk about friction and a relaxation time. (For an analytically solvable model illustrating these concepts, see [25].) The procedure just described will be applicable in practice only for especially simple systems or for systems with a finite number of degrees of freedom for which the required initial value calculation can actually be carried out. For such examples, the ''observed'' flow of energy from the collective to the noncollective degrees of freedom will show rapid fluctuations owing to the high frequency components of the motion associated with the intrinsic degrees of freedom. On the average, however, it will be unidirectional and thus correspond to an increase of entropy.

Thus the source of dissipation lies in the relative phase space associated with the intrinsic coordinates and not with the coarse-graining procedure introduced beginning with Eq. (5.19). The purpose of the latter is to reach a smooth macroscopic description of the dissipation, from which the fluctuations have been suppressed by averaging. The procedure consists of eliminating the intrinsic degrees of freedom from the equations of motion, going to the limit of a large number of such variables, assuming a suitable distribution in frequency (white noise) for the residual interaction between the collective and the noncollective coordinates, and then averaging. The final result is expressed in Eq. (5.40), which contains not only a frictional force of the conventional type, but additional contributions to the conservative forces arising from the coupling of the two spaces.

The arguments to be developed will be simplified considerably if we work only to the lowest nontrivial order in B^{ai}, V_a, and V_{ai}. This assumption is consistent with the procedure by which we shall define the canonical transformation from s_α, is_α^* to Q,P,q,p, which assumes that for good decoupling to occur, these quantities must be small. From Eqs. (5.6) and (5.7), we thereby deduce the equation

$$\ddot{q}_a = -\omega_a^2 q_a + X_a(Q), \tag{5.9}$$

$$X_a(Q) = -V_a - B_a^i V_i, \tag{5.10}$$

with solution

$$q_a(t) = q_a^{(h)}(t) + \int_0^t dt' \sin\omega_a(t-t')\frac{X_a(t')}{\omega_a}, \tag{5.11}$$

$$q_a^{(h)} = q_a(0)\cos\omega_a t + \frac{p_a(0)}{\omega_a}\sin\omega_a t. \tag{5.12}$$

Integrating by parts, we have

$$q_a(t) = q_a^{(h)}(t) + \frac{X_a(t)}{\omega_a^2} - \frac{X_a(0)}{\omega_a^2}\cos\omega_a t - \int_0^t dt' \cos\omega_a(t-t')\frac{\partial_i X_a(t')}{\omega_a^2}\dot{Q}^i(t'). \tag{5.13}$$

For the intrinsic momenta, we can derive the corresponding expression

$$p_a=\dot{q}_a^{(h)}-B^{ai}P_i+\int_0^t dt' X_a(t')\cos\omega_a(t-t'). \tag{5.14}$$

There is, naturally, no explicit sign of irreversibility in these equations. We now consider the assumptions that will lead to a simple (Markov) description of dissipation. For this purpose we must form the sums $V_{ia}q^a$ and $B^{ia}p_a$ that appear in Eqs. (5.5) and (5.4), respectively. At this point we find it convenient to replace these first-order equations by second-order equations. Working to only first order in $\dot{Q}^i$, we find with the help of Eqs. (5.5) and (5.7)

$$\ddot{Q}^i=B^{ij}\dot{P}_j+B^{ia}\dot{p}_a+\frac{\partial B^{ia}}{\partial Q_k}\dot{Q}^k p_a=F^i+F^{ia}q_a-G_k^{ia}\dot{Q}^k p_a, \tag{5.15}$$

$$F_i=-B^{ij}V_j-B^{ia}V_a, \tag{5.16}$$

$$F^{ia}=-B^{ij}V_{ja}-B^{ia}\omega_a^2, \tag{5.17}$$

$$G_k^{ia}=-\frac{\partial B^{ia}}{\partial Q^k}. \tag{5.18}$$

We infer from Eq. (5.15) that Q^i contains both the low frequencies of the collective motion and the high frequencies of the non-collective motion. For a macroscopic description of the collective motion, it is appropriate to coarse-grain in time. For this purpose, we assume that we can choose a time τ_O, which relative to a time τ_C, characteristic of the collective motion, and a time τ_{NC} characteristic of the intrinsic motion, satisfies the inequality

$$\tau_{NC}\ll\tau_O\ll\tau_C. \tag{5.19}$$

Under these conditions, if we average Eq. (5.15) over a time interval τ_O, the terms depending on the frequencies of the collective motion alone are essentially unaffected.

The existence of times satisfying Eq. (5.19) is subject to serious question, particularly because of the influence of avoided level crossings as the system evolves in shape space, i.e., as it traverses the collective manifold. But this problem also arises for the treatment of collective motion at zero temperature. The answer lies not in the single-particle spectrum but in the spectrum of the local harmonic equation derived in the next section. There is no basis for introducing the concept of collective motion for a system unless one or at most a few frequencies are low-lying and separated by a gap from the remaining frequencies. This gap, in the nuclear case, is unlikely to be more than an order of magnitude under optimum conditions, not leaving much room, it appears, for τ_O. We believe that it is incorrect, however, to associate the reciprocal of this gap with τ_{NC}. To obtain a conventional friction tensor, it is necessary to assume a very broad distribution of frequencies characterizing the interaction between the collective and the noncollective coordinates, peaked at a frequency which is more properly identified with $(1/\tau_{NC})$. The following derivations require that this assumption on time scales be valid.

To understand what happens to the high frequencies, we assume that $Q^i(t)$ can be written in the form

$$Q^i(t)=Q_0^i(t)+\delta Q^i(t). \tag{5.20}$$

This decomposition is defined by the requirement that the coarse-grain value of δQ^i vanish, which we write as

$$\langle\delta Q^i\rangle=0. \tag{5.21}$$

On the other hand to the order of accuracy to which we shall solve Eq. (5.15), i.e., to second order in the coupling between the collective and noncollective spaces we shall also need the value of

$$\langle\delta Q^i(t)\,\delta Q^j(t)\rangle\neq 0. \tag{5.22}$$

To evaluate Eq. (5.22) to the required accuracy, it suffices to take δQ^i in the form

$$\delta Q^i(t)=\sum_a\,[Q_{a+}^i(t)\exp(i\omega_a t)+\text{c.c.}], \tag{5.23}$$

where the $Q_{a+}^i(t)$ are slowly varying functions of t. [The expansion (5.23) is initially subject to the criticism that the frequencies ω_a depend on Q^i and therefore on t. It is, however consistent with our other assumptions to ignore the variation over an averaging time T_O.] Arguing that at any time these functions take values that are randomly distributed in magnitude and sign, we can compute the correlation (5.22) assuming that only coherent sums survive, namely,

$$\langle\delta Q^i(t)\,\delta Q^j(t)\rangle=\delta_{ij}\sum_a\,2|Q_{a+}^i|^2. \tag{5.24}$$

We shall need both Eqs. (5.21) and (5.24) for what follows. We note that the approximation

$$\dot{Q}^i(t)=\dot{Q}_0^i(t)+\sum_a\,(i\omega_a Q_{a+}^i(t)\exp(i\omega_a t)+\text{c.c.}), \tag{5.25}$$

which neglects $\dot{Q}_{a+}^i(t)$, will also be needed below.

Before entering into the details of the time-averaging process, it may serve the reader to remark that the end result of our manipulations is Eq. (5.41), which contains both conservative forces and frictional forces. As explained above, the source of friction does not lie in the time-averaging process *per se* but in the fact that there are many intrinsic degrees of freedom, and that energy initially in the collective motion will flow out (on the average) and not return to this mode in macroscopic time. What the averaging does is enforce a smooth description of this dissipative process. The conservative force is a sum of three types of contributions—the smooth given forces on the collective manifold, the smooth forces arising from the interaction of the collective modes with the low-frequency motion of the intrinsic coordinates, and the time-averaged effect of the high frequency fluctuations. Thus some effects of the high-frequency fluctuations are present, but how to connect this with our treatment of dissipation remains an open question.

We turn to the evaluation of the time average of Eq. (5.15), with the aid of Eqs. (5.13) and (5.14). It is this average which will be utilized for the study of the classical relaxation process. The values of Q^i_{a+} that enter in this calculation will be derived subsequently. Consider for example the term

$$F^i(Q)=F^i(Q_0)+\frac{\partial F^i}{\partial Q^j}\delta Q^j+\frac{1}{2}\frac{\partial^2 F^i}{\partial Q^j\partial Q^k}\delta Q^j\delta Q^k+\cdots. \tag{5.26}$$

When we average over t, utilizing Eqs. (5.21) and (5.24), we find that Eq. (5.26) reduces to

$$F^i\to F^i+F^i_{\text{fluc},1},$$

$$F^i_{\text{fluc},1}=\sum_j\frac{\partial^2 F^i}{\partial^2 Q^j}\sum_a|Q^j_{a+}|^2. \tag{5.27}$$

Here and below, it is understood that after the arrow the quantities that were functions of Q^i are now functions of Q^i_0, but we henceforth drop the subscript. The second term of Eq. (5.27) represents an additional contribution to the force arising from the high frequency fluctuations, since as we shall see below, the quantities Q^i_{a+} are driven by the amplitudes of the noncollective coordinates. Below, we shall find additional contributions having their origin in the high frequency fluctuations.

The evaluation of the next term of Eq. (5.15) yields the result

$$\begin{aligned}\sum_a F^{ia}q_a={}&\sum_a F^{ia}q_a^{(h)}+\sum_a\frac{F^{ia}X_a}{\omega_a^2}-\sum_a\frac{F^{ia}X_a(0)}{\omega_a^2}\cos\omega_a t\\&-\sum_a F^{ia}\int_0^t dt'\cos\omega_a(t-t')\frac{\partial_j X_a(t')}{\omega_a^2}\dot{Q}^j(t')\end{aligned} \tag{5.28}$$

$$\to F^i_{\text{fluc},2}+\delta F_i-\mathcal{F}^i_{j1}\dot{Q}^j. \tag{5.29}$$

Here the time averages of the first two terms of Eq. (5.28), which follow by arguments already given, are represented by the expressions

$$F^i_{\text{fluc},2}=\sum_a 2\partial_j F^{ia}[Q^j_{a+}q^{(h)}_{a-}(0)+\text{c.c.}], \tag{5.30}$$

$$\delta F^i=\sum_a\frac{F^{ia}X_a}{\omega_a^2}, \tag{5.31}$$

$$q^{(h)}_{a-}(0)=\frac{1}{2}\left(q_a^{(h)}(0)+i\frac{p_a^{(h)}(0)}{\omega_a}\right). \tag{5.32}$$

Remembering that we are working only to the second order in the collective-noncollective coupling the time average of the third term vanishes, since the quantity $F^{ia}X_a(0)$, evaluated at Q_0, is already of this order. Finally we must consider the origin of the friction term, which requires an additional argument.

To extract a frictional term without memory, we proceed as follows. We assume that we can replace the sum over a by an integral over ω,

$$\sum_a F^{ia}(t)\frac{\partial_j X_a(t')}{\omega_a^2}\to\int d\omega\Phi^i_j(\omega,t,t'), \tag{5.33}$$

where Φ^i_j, though necessarily an integrable distribution, is a very broad, slowly varying function of ω. For the purposes of evaluating the integral over ω (which we now do first),

$$I^i_j(t,t')\equiv\int_0^\infty d\omega\cos\omega(t-t')\Phi^i_j(\omega,t,t'), \tag{5.34}$$

we further assume that we can treat Φ^i_j as a function, $A^i_j(t,t')$, of the times alone (white noise assumption). To this approximation we have

$$I^i_j=\pi A^i_j(Q(t))\delta(t-t'). \tag{5.35}$$

From these considerations, we then conclude that [26]

$$\mathcal{F}^i_{j1}(Q)=\frac{1}{2}\pi A^i_j(Q). \tag{5.36}$$

We have finally to consider the last term in Eq. (5.15), in which we insert Eq. (5.14) Discarding a term of second order in the collective velocity, we have

$$\begin{aligned}-\sum_a G^{ia}_j\dot{Q}^j p_a={}&-\sum_a G^{ia}_j\dot{Q}^j\bigg[\dot{q}_a^{(h)}(t)\\&+\int dt'\cos\omega_a(t-t')X_a(t')\bigg]\end{aligned} \tag{5.37}$$

$$\to F^i_{\text{fluc},3}-\mathcal{F}^i_{j2}\dot{Q}^j. \tag{5.38}$$

Here $\mathcal{F}^i_{j2}$ can be defined in analogy to $\mathcal{F}^i_{j1}$, Eq. (5.36), and

$$F^i_{\text{fluc},3}=-\sum_a G^{ia}_j\omega_a^2(Q^j_{a+}q^{(h)}_{a-}(0)+\text{c.c.}). \tag{5.39}$$

Collecting results we obtain our final form for the collective equations of motion

$$\ddot{Q}^i=F^i+\delta F^i+F^i_{\text{fluc}}-\mathcal{F}^i_j\dot{Q}^j, \tag{5.40}$$

where the first term on the right-hand side of Eq. (5.40) is defined by Eq. (5.16), the second by Eq. (5.31), the third is a sum of three terms given by Eqs. (5.27), (5.30), and (5.39), and the dissipative term is a sum of two terms defined in Eqs. (5.36) and (5.38). In addition to the frictional force, which was expected, we see that there are two contributions of second order in the coupling between the collective and the noncollective spaces that contribute to the conservative force. One of these, F^i_{fluc}, depends on the initial conditions for the noncollective variables, more particularly on three quadratic forms in these values.

If we write Eq. (5.40) in the form (B_{ij} is the mass matrix inverse to B^{ij})

$$B_{ij}\ddot{Q}^j=-\partial_i\mathcal{V}-\mathcal{F}_{ij}\dot{Q}^j, \tag{5.41}$$

$$\mathcal{F}_{ij}=B_{ik}\mathcal{F}^k_j, \tag{5.42}$$

thus defining the potential energy, $\mathcal{V}$, of the conservative forces, we can associate the expression

$$E_M = \frac{1}{2} B_{ij} \dot{Q}^i \dot{Q}^j + \mathcal{V}(Q) \tag{5.43}$$

with the mechanical energy of collective motion. The dissipative terms proportional to $\mathcal{F}$ lead to a loss of mechanical energy for which we obtain the standard energy-flow equation

$$\dot{E}_M = -\mathcal{F}_{ij} \dot{Q}^i \dot{Q}^j. \tag{5.44}$$

It remains only to show that the first-order Fourier coefficients, $Q^i_{a+}(t)$ are proportional to $q^{(h)}_{a+}(0)$. In fact, it is straightforward to derive in lowest order from Eq. (5.15) the equation

$$-\omega_a^2 Q^i_{a+} = -\Omega^i_j Q^j_{a+} + L^{ia} q^{(h)}_{a+}(0), \tag{5.45}$$

$$\Omega^i_j = -\partial_j F^i, \tag{5.46}$$

$$L^{ia} = F^{ia} + i\omega_a G^{ia}_j \dot{Q}^j. \tag{5.47}$$

Formally, we have therefore

$$Q^i_{a+} = \left(\frac{1}{\boldsymbol{\Omega} - \omega_a^2} \right)^i_j L^{ja} q^{(h)}_{a+}(0). \tag{5.48}$$

The solution (5.48) can be made more explicit by diagonalizing the matrix $\boldsymbol{\Omega}$.

The study of Eq. (5.40) for some simplified models is under way. As it stands this equation is not yet well-defined as a macroscopic equation, since F^i_{fluc} depends on a given set of initial conditions for the noncollective coordinates. To have a result that depends only on the collective coordinates, we shall have to introduce a further averaging over a distribution of initial conditions of the noncollective coordinates (or, more pragmatically, incorporate the fluctuation force phenomenologically into δF^i). The quantities needed for the computation of the results developed in this section are all obtainable, in principle, from the theory explained in Sec. VI. Actually carrying through the manipulations for a realistic model would seem to require some simplifying assumptions for the distribution of matrix elements coupling collective and noncollective variables.

Given $Q^i(0)$ and $\dot{Q}^i(0)$, Eq. (5.41) allows us to discuss the relaxation of the collective mechanical degrees of freedom. Here we must remember that the macroscopic parameters in this equation also depend on the occupation numbers, and therefore the problem is not well defined as an initial-value problem until we adjoin the equations of motion for the latter, the so-called master equations. We have already mentioned the two special cases of master equations that can be treated with relative ease. If we assume that the occupation numbers remain fixed, we are studying what we define as one-body friction. The other case considered, in which the system relaxes through a sequence of states of local equilibrium, can be considered the strong-collision limit. Further discussion of these scenarios will be found in Sec. VI.

VI. DECOMPOSITION OF MEAN-FIELD HAMILTONIAN INTO COLLECTIVE AND NONCOLLECTIVE PARTS

The considerations of the previous subsection were based on transformation of the mean-field Hamiltonian into the form (5.3) together with the associated equations of motion (5.4)–(5.7). In this section we describe how this transformation can be effected. The procedure is an extension of the calculations carried out at zero temperature, as we shall describe. As has already been emphasized, the transformation will be based on the identity

$$H(Q,P,q,p,n_a) = W(s_\alpha(Q,P,q,p), s^*_\alpha, n_a). \tag{6.1}$$

To determine the transformation implied by Eq. (6.1), we could invoke the full machinery of LACM described in Refs. [3,4]. In the following, however, we shall utilize an approximate form of one of the methods described in these references, the local harmonic approximation (LHA), which is fully described below.

The procedure is to reexpress the equations of motion (4.7) by writing for the left-hand side

$$\dot{s}_\alpha = [\dot{Q}^i \partial_{Q^i} + \dot{P}_i \partial_{P_i} + \dot{q}^a \partial_{q^a} + \dot{p}_a \partial_{p_a}] s_\alpha \tag{6.2}$$

and then substituting in this expression the equations of motion (5.4)–(5.7). On the right-hand side of Eq. (4.7), we expand in powers of $P^k q^l p^m$, with $k+l+m \leqslant 1$ and then equate corresponding powers on both sides. The resulting set of equations contains the density matrix nonlinearly. However, for the determination of the off-diagonal density matrix and of its first derivatives with respect to Q and P at a given point, the equations derived thus far do not suffice. The necessary additional equations are provided by differentiating the equation of motion with respect to Q^i (n_a fixed) and afterwards setting $P=Q=p=0$. In order to obtain closure from this step, we must, in general, ignore second derivatives of s_α. The resulting set of equations then contains only zeroth and first derivatives of the density matrix. By extending these considerations, a procedure can be formulated for including second and higher derivatives. (Under the special circumstances of a point canonical transformation, we have even shown [3], using established geodesic properties of a decoupled manifold, how to eliminate the second derivatives that occur in favor of the first derivatives, and thus obtain closure at this point. We shall not pursue this possibility here.)

Let us now recall the role of the master equations in our approach. Together with Eq. (5.41) they determine how, with a given set of initial conditions for n_a and for the mechanical variables, the system will move through a subspace of the collective manifold. Any special choice of master equations is covered by these remarks. However, for the two special scenarios that we have proposed, the limits of weak and strong collisions, the possible set of points that can be traversed in the collective manifold is preassigned to a one-dimensional subspace of the occupation number space. In fact this was one of the principal motivations for introducing these special cases. It allows us to evade the impossibly difficult task of constructing the entire collective manifold and to replace it by a feasible calculation, albeit a different one in detail for the two special cases. We shall return below to a further elaboration of this point.

Returning to the technical development, we introduce the definitions

$$\partial_i = \partial_{Q^i}, \tag{6.3}$$

$$\partial_a = \partial_{q^a}, \tag{6.4}$$

$$\partial^i = \partial_{P_i}, \tag{6.5}$$

$$\partial^a = \partial_{p_a}, \tag{6.6}$$

$$\partial_0 = -V_i \partial^i - V_a \partial^a, \tag{6.7}$$

$$\partial^{1i} = B^{ij}\partial_j + B^{ia}\partial_a, \tag{6.8}$$

$$\partial^{1a} = B^{aj}\partial_j + B^{ab}\partial_b, \tag{6.9}$$

$$\partial_{2i} = -V_{ij}\partial^j - V_{ib}\partial^b, \tag{6.10}$$

$$\partial_{2a} = -V_{aj}\partial^j - V_{ab}\partial^b. \tag{6.11}$$

In terms of these definitions, we now record the equations, (6.12) and (6.13), that follow from the expansion described in the second paragraph of this section plus the additional set, Eq. (6.14), needed for the formulation of a local harmonic algorithm,

$$\partial_0 s_\alpha = -i\frac{\partial W}{\partial s_\alpha^*} \equiv -iS_\alpha, \tag{6.12}$$

$$\partial^{1\mu} s_\alpha = -i[M_{\alpha\beta}\partial^\mu s_\beta + L_{\alpha\beta}\partial^\mu s_\beta^*], \tag{6.13}$$

$$\partial_{2\mu} s_\alpha = -i[M_{\alpha\beta}\partial_\mu s_\beta + L_{\alpha\beta}\partial_\mu s_\beta^*], \tag{6.14}$$

$$M_{\alpha\beta} = \frac{\partial^2 W}{\partial s_\alpha^* \partial s_\beta}, \tag{6.15}$$

$$L_{\alpha\beta} = \frac{\partial^2 W}{\partial s_\alpha^* \partial s_\beta^*}, \tag{6.16}$$

where it is understood that all quantities are functions only of Q and of the occupation numbers, and in which we have combined the sets i and a into a single index set μ. To the above we adjoin the complex conjugate set. Explicit formulas for S,M,L are given in Appendix C.

We now ask what, if anything, is actually determined by the above set of equations. Without further restriction they are identities (to linear order in all variables but Q) satisfied by *any* canonical transformation from the original to the new set of canonical variables. For example, any transformation satisfying the Lagrange bracket conditions

$$\partial_\mu s_\alpha \partial^\nu s_\alpha^* - \partial^\nu s_\alpha \partial_\mu s_\alpha^* = -i\delta_\nu^\mu, \tag{6.17}$$

$$\partial_\mu s_\alpha \partial_\nu s_\alpha^* - \partial_\nu s_\alpha \partial_\mu s_\alpha^* = 0, \tag{6.18}$$

$$\partial^\mu s_\alpha \partial^\nu s_\alpha^* - \partial^\nu s_\alpha \partial^\mu s_\alpha^* = 0, \tag{6.19}$$

will automatically guarantee the satisfaction of Eqs. (6.12)–(6.14).

What we actually want is a canonical transformation that minimizes the coupling between the collective and the noncollective spaces. For the spectroscopic problem studied previously, the object was clearly to obtain, upon quantization, a Hamiltonian describing a well-developed collective spectrum, weakly coupled to the remaining Hilbert space. For the transport problem studied in this work, minimizing the coupling between collective and noncollective spaces allows us to treat dissipation by perturbative means. The decoupling requirement, when translated into the quantitative terms reviewed below defines the collective manifold. The latter is a geometrical object; the choice of a coordinate system is initially a matter of numerical convenience. For example, in the treatment of the low-energy spectrum of ^{28}Si [4], our *a priori* prejudice was that the collective coordinate should strongly resemble the quadrupole moment. However, the algorithm used to solve the problem produces a ''dressed'' collective variable that is a mixture of multipoles of even order. Nevertheless, when the calculation is done, we have a single-particle density matrix defined over the collective manifold, and thus we can calculate any one-particle physical quantity of interest.

At zero temperature, the decoupling requirement dictated the further imposition on the transformation of the so-called first order decoupling conditions [3]. These are the conditions that the terms in the classical Hamiltonian (5.3) linear in q and p vanish, namely,

$$V_a(Q) = \partial_a W = [\partial_a s_\alpha \partial_{s_\alpha} + \partial_a s_\alpha^* \partial_{s_\alpha^*}]W = 0, \tag{6.20}$$

$$B^{ai} = \partial^a \partial^i W = 0. \tag{6.21}$$

Because of the complete analogy in the Hamiltonian structure, we now argue that the same conditions provide an extension of the zero temperature theory to finite excitation energy. What we must admit is the additional complication that arises from the fact that the collective manifold depends not only on the collective coordinates Q but on the assigned values of the occupation numbers. At zero temperature, the occupation distribution is that of a Fermi sphere. This distribution remains fixed as we map out the dependence of the collective manifold on Q, though at each point the Fermi distribution refers to a different basis of single-particle states.

In the local harmonic method, the construction of the collective manifold at an arbitrary value of Q involves an iteration between Eq. (6.12) and the local harmonic equations (6.13) and (6.14), both simplified by the conditions (6.20) and (6.21). This procedure, as described, for example, in Ref. [4], is initiated at the point of dynamic equilibrium, where the constrained Hartree-Fock conditions reduce to the unconstrained limit and decouple from the local harmonic equations. We thus have at this limit an ordinary Hartree-Fock calculation and a separate random phase approximation (RPA) calculation. The solution at this point provides the starting values for an iterative treatment for a nearby nonequilibrium value. Continuing in this manner, we bootstrap our way from point to point.

For the corresponding problem for finite excitation energies, it is natural to choose a point of thermodynamic equilibrium as a starting point. At such a point the problem reduces to the solution of separate standard thermal Hartree-

Fock and thermal RPA problems [27–30]. We suppose that the system has been put into contact with a heat bath to fix the initial temperature. We thus obtain a starting set of occupation numbers of the form (4.14).

If we now move away from equilibrium to construct a general manifold suitable for the study of transport phenomena, we face a general problem of daunting proportions if we wish to obtain the dynamical parameters for arbitrary values of occupation numbers. For this reason, as already emphasized, we have chosen to study two limiting cases of possible physical interest, each corresponding to a one-dimensional subspace of the space of occupation numbers. One limit is that of collisionless motion, corresponding to fixed occupation numbers (in the local coordinate system) and one-body friction. For this case, the formal problem is the same as at zero excitation energy, since we deal with a case of fixed occupation numbers as we explore changes of the collective variables. The set of occupation numbers is that determined at equilibrium at a fixed temperature. The resulting manifold is thus constructed from a series of collective paths with fixed entropy. Technically, this problem is more difficult than the zero-temperature problem because of the increase in the number of degrees of freedom of the Hamiltonian system.

The other limit is that of two-body collisions establishing local thermodynamic equilibrium on a time scale small compared to that associated with the collective motion. For this limit it is convenient, technically, to calculate collective paths at fixed T, where each point is associated with an occupation number distribution of the type (4.14). We start the calculation again at a point of thermal equilibrium, now keeping T fixed as we change Q. [This calculation is not to be confused with what happens in an actual relaxation process, where T will change with time, as forced in part by Eq. (4.18).] Thus, as opposed to the collision-less regime, we want the solutions of the LHA only at points where the occupation numbers satisfy Eq. (4.14), with local values of single-particle energies and chemical potential, adjusted as part of the calculation.

The submanifold of occupation numbers for which we construct solutions can be thus be characterized as follows. In the collisionless case we have, zero referring to equilibrium,

$$n_a = n_a(Q_0, T_0). \tag{6.22}$$

Since $Q_0 = Q_0(T_0)$, this is a one-dimensional subspace with a given entropy. In the strong collision limit

$$n_a = n_a(Q, T), \tag{6.23}$$

is the Fermi distribution (4.14). The derivation of the latter by maximization of the local entropy guarantees that for each Q, we have replaced the set n_a by the single variable, T, defining the local equilibrium. In principle (though not in practice) nothing prevents us from calculating the entire manifold of canonical transformations and then identifying the two special subspaces afterwards.

Before continuing with the technical details, the most important additional point to keep in mind is that after we complete the algorithm to be described below the solution found will not, in general, satisfy the decoupling conditions (6.20) and (6.21) exactly (except for the singular case of exactly decoupled motion when there is no dissipation). As explained below, the transformation found will, however, allow the evaluation of the quantities that occur in these conditions. Their non-vanishing values are, as we have seen in the previous section, essential to the development of dissipative behavior. Thus all the quantities in the Hamiltonian (5.3) can be evaluated.

The formulas required are obtained by inserting the solutions for the density matrix and its various first derivatives into an expansion of the right hand side of Eq. (6.1). The simplest example of such a calculation is the potential energy

$$V(Q) = W(s_\alpha(Q,0,0,0), s_\alpha^*, n_a). \tag{6.24}$$

Next in complexity is the first derivative

$$V_a(Q) = \partial_a W = \frac{\partial W}{\partial s_\alpha}\partial_a s_\alpha + \text{c.c.}, \tag{6.25}$$

where the right-hand side is evaluated at $P=q=p=0$. The remaining parameters that we need are all second derivatives,

$$B^{\mu\nu} = \partial^\mu \partial^\nu W \cong \frac{\partial^2 W}{\partial s_\alpha \partial s_\beta}\partial^\mu s_\alpha \partial^\nu s_\beta + \frac{\partial^2 W}{\partial s_\alpha \partial s_\beta^*}\partial^\mu s_\alpha \partial^\nu s_\beta^* + \text{c.c.}, \tag{6.26}$$

where we have (consistently) neglected second derivatives of the density matrix. In order to evaluate Eq. (6.25) and all the elements of Eq. (6.26), it is evident that we need all the solutions of the LHA equations (6.13) and (6.14), and not only the collective ones that play a special role in the self-consistent calculation.

We review briefly the properties and solutions of Eqs. (6.12)–(6.14). When the decoupling conditions are enforced, these equations simplify to the forms

$$-V_i \partial^i s_\alpha = -i S_\alpha, \tag{6.27}$$

$$B^{ij}\partial_j s_\alpha = -i[M_{\alpha\beta}\partial^i s_\beta + L_{\alpha\beta}\partial^i s_\beta^*], \tag{6.28}$$

$$-V_{ij}\partial^j s_\alpha = -i[M_{\alpha\beta}\partial_i s_\beta + L_{\alpha\beta}\partial_i s_\beta^*]. \tag{6.29}$$

They can be simplified further by the consistent assumptions that M and L are real symmetric matrices and that the partial derivatives are either real or imaginary,

$$\partial_i s_\alpha^* = \partial_i s_\alpha, \tag{6.30}$$

$$\partial^i s_\alpha^* = -\partial^i s_\alpha. \tag{6.31}$$

This allows us to eliminate the partials of s_α^*. The formalism now consists of the constrained Hartree-Fock equation (6.27) and two equivalent eigenvalue equations obtained by combining (6.28) and (6.29), of which one is

$$-(VB)_i^j \partial_j s_\alpha = [(L-M)(L+M)]_{\alpha\beta}\partial_i s_\beta, \tag{6.32}$$

and the other, for $\partial^i s_\alpha$, is the transpose of Eq. (6.32). This implies that VB and BV have the same diagonal form (if there are no degeneracies, as we assume). These eigenvalue equations plus the corresponding Lagrange bracket conditions are equivalent to the eigenvalue problem of the thermal RPA [27–30], but in our case the theory applies outside of thermal equilibrium.

As emphasized previously, the solution of the system obtained utilizes an algorithm of the same general structure as required at zero temperature, a procedure that has been described in considerable detail in our previous work [4] and will not be repeated here. The solutions of the eigenvalue problem automatically satisfy the homogeneous Lagrange bracket equations, whereas the inhomogeneous brackets provide normalization conditions. The solution procedure is usually started at a point of thermal equilibrium where the Hartree-Fock equations decouple from local harmonic equations. At a general point, the algorithm requires an iteration between the constrained Hartree-Fock equations and the eigenvalue equations. This is the essence of the local harmonic approximation.

As remarked earlier, we are confining our attention to two cases. If, starting from equilibrium, we keep the occupation numbers constant as we change Q, the analogy with the calculation at zero temperature is rather complete. If, on the other hand we keep the temperature fixed, at every point there is the additional task of finding self-consistent values of the occupation numbers. This type of calculation was also required for thermal Hartree-Fock. As a final observation, as we have implied all along, it is possible to move out from the one-dimensional subspaces of fixed occupation numbers, in effect to change n_a for fixed Q. We first set

$$\frac{\partial W(s_\alpha,s_\alpha^*,n_a)}{\partial n_a}=\frac{\partial H}{\partial n_a}, \tag{6.33}$$

where W is the full Hartree-Fock energy and H is the classical expression (5.3). Equating powers of P, p, and q on both sides of this equation yields microscopic expressions for the first derivatives of the various force and mass coefficients with respect to n_a. Such formulas could be used to extend the study of the relaxation problem away from the limiting scenarios.

We summarize the argument developed in this section. Given the mean-field Hamiltonian at finite excitation energy, we have described a method for introducing an optimal decomposition of the total space into collective and noncollective coordinates. In general these spaces will not be exactly decoupled, but as a result of the actual calculations, we can evaluate the coupling terms. In other words, we can find explicit forms of Eqs. (5.4)–(5.7) and from these project out the collective subspace that leads to a dissipative dynamics, the procedure described in detail in Sec. V.

VII. SUMMARY AND PERSPECTIVE

In this work, we have introduced a new method for the study of large amplitude collective motion, including dissipation, in an extended Born-Oppenheimer approximation. Though to start with it is a quantum formulation that carries us outside the framework of mean field theory, we have up to the present worked out the details only within the (extended) boundaries of mean field theory. This means that we have neglected two-body dissipation, though we anticipate that the methods developed can be extended to include this case.

The practical end of our labors is a set of classical equations of motion (5.41) for the collective coordinates that includes necessary dissipative parameters to describe the relaxation of a perturbed collective subsystem and the leakage of energy to the noncollective degrees of freedom. We consider this equation now for a single collective coordinate,

$$B(Q,n_a)\ddot{Q}+\mathcal{F}(Q,n_a)\dot{Q}+\partial_Q V(Q,n_a)=0. \tag{7.1}$$

This looks like an ordinary Newton equation with a friction term, except that the macroscopic parameters $B,\mathcal{F}$ depend on the value of the collective coordinate, and there is a residual quantum aspect in that they also depend on a set of occupation numbers of single-particle orbitals. There are two aspects of this equation that have been discussed. How does one derive it? How does one use it?

By far the major part of the discussion has been devoted to the first question. Consider a fixed set of n_a. (At zero temperature, these are the usual values 1 and 0 defining a Slater determinant. At finite excitation energy, the first choice is a set of occupation numbers for equilibrium at some finite temperature.) For such a single choice, the determination of V and B, as described in Sec. VI is in its essentials the same as at zero temperature, as summarized by the phrase local harmonic approximation. This allows us to calculate the first line of the transformed Hamiltonian, Eq. (5.3). If we are interested in leading corrections, we also calculate the second line. But in previous work we have ignored the existence of the third line which describes the coupling between the collective and the noncollective degrees of freedom, that will be non-zero unless there is exact decoupling. To include both the second and third lines, we need a complete set of solutions of the local RPA equation (6.32). For example, given such solutions, $V_a(Q)$ can be calculated from Eq. (6.20) and there are corresponding formulas for the other quantities needed in the subsequent development.

At this point, we could, for a fixed set of n_a simply study the classical equations of motion (5.4)–(5.7) as an initial value problem. Of most interest would be the case that the initial energy is all in the collective motion. This study is feasible if the total number of degrees of freedom is not too great. [We are undertaking such a program for models in which the (Q,P,q,p) basis is known.]

On the other hand, Eq. (5.41) refers only to a very special limiting case in which the interaction strength between collective and noncollective degrees of freedom is distributed over a very broad spectrum of oscillator energies, one that can be approximated by white noise. There is no guarantee that a chosen model will have such a property, though again we may choose to study one in which such a property is imposed. What is involved in the calculation of the frictional force can be seen most simply if we ignore the fluctuation analysis that consumes much of Sec. V. Then for the purposes of calculating $\mathcal{F}$, the essential steps associated with obtaining the consequences of the white-noise assumption are Eqs. (5.33)–(5.37). From these we see that at least in principle $\mathcal{F}$ can be obtained from an *ab initio* calculation.

Given Eq. (5.41), how then do we use it? The simplest case is that of true one-body friction. Here the large manifold of values of (Q,n_a) is indeed restricted to a two-dimensional manifold of values where $n_a=n_a(T)$, with T a set of equilibrium values of the temperature. Disturbances away from equilibrium are assumed to take place with fixed n_a, i.e., at constant entropy. Here Eq. (5.41) by itself defines an initial-value problem. We have also described a relatively accessible second case in which relaxation occurs through points of local thermodynamic equilibrium. Here the solution of the relaxation problem requires the joint consideration of Eq. (5.41) and of Eq. (4.18), describing how the local temperature changes with time. Studies of these two cases for simple models are in progress.

The formalism developed in this paper allows in principle an extended scenario in which we would couple Eq. (5.41) with a more general equation for the time rate of change of the occupation numbers (master equations), either phenomenological or involving a Boltzmann-Uhlenbeck collision term. A major complication is that we would have to study the collective manifold over a multidimensional space of the n_a, though we might try at first to limit ourselves to a small neighborhood of one of the limiting cases. Beyond that would be the inclusion of two-body friction.

ACKNOWLEDGMENTS

This research was started at a workshop on collective motion at the Institute of Nuclear Theory at the University of Washington. The authors would like to thank members of the INT for their hospitality. They also wish to acknowledge many useful discussions with N. R. Walet during the course of this work. The Laboratoire de Physique Théorique et Hautes Energies is a Laboratoire associé au C.N.R.S., URA 0063.

APPENDIX A: FURTHER DISCUSSION OF THERMAL STATES. RELATION TO THERMOFIELD THEORY

The thermal state has a remarkable similarity to the state in thermofield theory, see, e.g., [31]. The thermofield theory can be summarized as follows: One produces a copy of the Hilbert space $\mathcal{G}$ with states $|\psi\rangle$ yielding the $\tilde{\mathcal{G}}$ space with states $|\tilde{\psi}\rangle$. The full space is the product $\mathcal{G}\otimes\tilde{\mathcal{G}}$. A basis in the full space can be constructed from the product states

$$|n,\tilde{n}\rangle\rangle=|n\rangle\otimes|\tilde{n}\rangle, \tag{A1}$$

and a general state is expanded as

$$|\Psi\rangle\rangle=\sum_{n\tilde{n}} c_{n\tilde{n}}|n,\tilde{n}\rangle\rangle. \tag{A2}$$

Consider now an observable from the physical Hilbert space, $\hat{A}\in\mathcal{G}$. Its expectation value becomes

$$\langle\langle\Psi|\hat{A}|\Psi\rangle\rangle=\sum_{nn'} D_{nn'}\langle n'|\hat{A}|n\rangle, \tag{A3}$$

$$D_{nn'}=\sum_{\tilde{n}} c_{n\tilde{n}}c^{*}_{n'\tilde{n}}, \tag{A4}$$

where it is obvious how the averaging over $\tilde{\mathcal{G}}$ space produces a mixed ensemble $D_{nn'}$ in $\mathcal{G}$ space. The expectation value holds for every observable $\hat{A}$. Thus the formalism utilizing the states $|\Psi\rangle\rangle$ of the thermofield theory is equivalent to the standard formalism of the density matrix

$$\hat{D}=\widetilde{\mathrm{tr}}\{|\Psi\rangle\rangle\langle\langle\Psi|\}=|n\rangle\sum_{\tilde{n}} c_{n\tilde{n}}c^{*}_{n'\tilde{n}}\langle n'|=|n\rangle D_{nn'}\langle n'|, \tag{A5}$$

where $\widetilde{\mathrm{tr}}$ means the trace over the $\tilde{\mathcal{G}}$ space. This indicates that all three pictures, thermal states, thermofield theory, and density matrices are equivalent.

Next we try to express the collective decoupling in the thermofield representation. The collective space is doubled $|Q,\tilde{Q}))=|Q)\otimes|\tilde{Q})$ and similarly for the intrinsic space. A pure intrinsic state (temperature 0) would then read

$$|Q,\tilde{Q}))|f,\tilde{f}]]=|Q,\tilde{Q}))|f]\otimes|\tilde{f}], \tag{A6}$$

and a mixed state becomes

$$|\Psi\rangle\rangle=|Q,\tilde{Q}))\sum_{f\tilde{f}} a_{f\tilde{f}}|f]\otimes|\tilde{f}]. \tag{A7}$$

The expectation value in this thermofield state becomes

$$\langle\langle\Psi|\hat{A}|\Psi\rangle\rangle=\mathrm{tr}\{\hat{A}|Q)\hat{d}(Q|\}, \tag{A8}$$

$$\hat{d}=|f]d_{ff'}[f'|, \tag{A9}$$

$$d_{ff'}=\sum_{\tilde{f}} a_{f\tilde{f}}a^{*}_{f'\tilde{f}}, \tag{A10}$$

which is exactly the expectation value in the thermal state. We thus can establish the equivalence

$$|Q)\sum_{ff'} |f]a_{ff'}[f'|\equiv|Q,\tilde{Q}))\sum_{f\tilde{f}} a_{f\tilde{f}}|f,\tilde{f}]]. \tag{A11}$$

This equivalence encourages the following set of observations.

(1) It links the new development of the ‘‘thermal states’’ to the old and well settled concept of thermofield theory. This gives confidence that the present thermal representation is useful and reasonable.

(2) It shows that the ‘‘thermal states’’ are fully equivalent to density matrices because this equivalence has been established long ago for the thermofield states. It is a matter of taste and experience which of the various representations one prefers. The thermal states look closer to pure states and thus allow one to work out all steps in sort of a Hilbert space picture.

(3) The ‘‘thermal states’’ seem to be simpler because one does not need to double the Hilbert space. But this limits the range of applicability, as shown by the following points.

(4) The ‘‘thermal state’’ $|Q)\hat{d}^{1/2}$ cannot be used in a linear superposition, as, e.g., $\int dQ|Q)\hat{d}^{1/2}g(Q)$, because the $\hat{d}^{1/2}$ is related to a bilinear object. Thus the ‘‘thermal states’’ are used in this work only as a pathway to a *semiclassical dynamics* where one has only one Q at one time, i.e., in a dynamics which is expressed solely in terms of $Q(t)$, etc.

APPENDIX B: ALTERNATIVE PRESENTATION OF GENERALIZED KERMAN-KLEIN METHOD FOR FINITE TEMPERATURE

In the body of the paper we have developed a version of a generalized symmetry-preserving equation of motion method for mixed states, applicable to transport phenomena as well as to thermal equilibrium. In the brief account included here, we describe an older previously unpublished argument for such a generalization restricted to the case of thermal equilibrium.

Let X be an arbitrary operator. We contrast four physical situations.

For the study of the ground state, $|0\rangle$ at $T=0$, the relevant quantity is

$$\langle 0|X|0\rangle = \mathrm{tr}\, X\mathcal{P}_0,$$
$$\mathcal{P}_0 = |0\rangle\langle 0|. \tag{B1}$$

For the study of thermal equilibrium at finite temperature we replace Eq. (B1) by (grand canonical ensemble)

$$\langle X\rangle = \frac{\mathrm{tr}\, X \exp(-\beta H')}{\mathrm{tr}\exp(-\beta H')},$$
$$\equiv \mathrm{tr}\, XD,$$
$$H' = H - \mu N. \tag{B2}$$

Though usually left unspecified, this formulation contains the assumption that the transfer of any energy to the system raises its temperature.

By contrast the Kerman-Klein theory contains the implicit assumption that we are dealing with a system that boasts an ensemble of cold (collective) states described by a Hamiltonian H_C and labeled $|A\rangle, |B\rangle, \ldots$. The fundamental role is played by the transition matrix element

$$\langle B|X|A\rangle = \mathrm{tr}\, X\mathcal{P}_{AB},$$
$$\mathcal{P}_{AB} = |A\rangle\langle B|. \tag{B3}$$

A comparison between Eqs. (B3) and (B1) *suggests* that an appropriate generalization of Eq. (B2) is

$$\langle\langle B|X|A\rangle\rangle \equiv \mathrm{tr}\, X D_A^{1/2} D_B^{1/2},$$
$$D_A = \frac{\exp[-\beta(H - H_C - \mu_A N)]\mathcal{P}_A}{\mathrm{tr}\exp[-\beta(H - H_C - \mu_A N)]\mathcal{P}_A}. \tag{B4}$$

Here D_A is a mixed state that is pure with respect to the collective state $|A\rangle$ (whose projection operator is $\mathcal{P}_A$ and whose chemical potential is μ_A) and a grand canonical ensemble with respect to noncollective excitations. Since it is a positive definite operator, a positive square root is a well-defined concept.

To use these last ideas in the equations of motion, we define a thermal single particle density matrix

$$\rho(\alpha A|\beta B) = \mathrm{tr}\, a^*_\beta a_\alpha D_A^{1/2} D_B^{1/2}. \tag{B5}$$

The thermal version of the Kerman-Klein equations follows from the assumption of the validity of the factorization

$$\mathrm{tr}\, a^*_\gamma a^*_\delta a_\alpha a_\beta D_A^{1/2} D_B^{1/2} \cong \frac{1}{2}[\rho(\beta A|\gamma C)\rho(\alpha C|\delta B) - (\gamma\leftrightarrow\delta) - (\alpha\leftrightarrow\beta) + (\gamma\leftrightarrow\delta, \alpha\leftrightarrow\beta)], \tag{B6}$$

which can, as in the text, be augmented into a formally exact expression. The present construction, though sufficient for the formulation of an equilibrium statistical mechanics, is not as general as that proposed in the body of the paper.

APPENDIX C: EXPLICIT FORMULAS FOR THE LOCAL HARMONIC APPROXIMATION

In this Appendix, we give explicit formulas for the quantities S, L, and M that appear in Eqs. (6.12)–(6.16) and play an essential role in the formulation of the local harmonic approximation. These quantities can be evaluated starting from the mean-field Hamiltonian using formulas given in Sec. IV. Notice that the index α actually refers to a pair (b,a), $b>a$. Recalling, in particular, the definitions (6.15) and (6.16), we find

$$S_{ba} = \sqrt{n_a - n_b}\,\mathcal{H}_{ba}, \tag{C1}$$

$$M_{badc} = M^*_{dcba} = \frac{1}{\sqrt{(n_a - n_b)(n_c - n_d)}}[\mathcal{H}_{bd}\delta_{ca}(n_c - n_b) - \mathcal{H}_{ca}\delta_{db}(n_a - n_d)] + V_{bcad}\sqrt{(n_a - n_b)(n_c - n_d)}, \tag{C2}$$

$$L_{badc} = L_{dcab} = \frac{1}{2\sqrt{(n_a - n_b)(n_c - n_d)}}[\mathcal{H}_{da}\delta_{cb} - \mathcal{H}_{bc}\delta_{da}] \times [(n_a - n_b) - (n_c - n_d)] + V_{dbac}\sqrt{(n_a - n_b)(n_c - n_d)}. \tag{C3}$$

It is easily seen that in the zero temperature limit, when the occupation numbers correspond to the choice $(b,a) \rightarrow (ph)$, $n_p = 0, n_h = 1$, that the matrices reduce to pieces of the well-known RPA matrix, M to the Tamm-Dancoff (shell-model) matrix and L to a two-particle, two-hole matrix element of V, associated with the inclusion of ground-state correlations.

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