Revised generalized density matrix method for the study of nuclear collective motion

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(Received 13 January 1984)

A common flaw in the theoretical structure of the generalized-Hartree-Fock approximation of Kerman and Klein and of the equivalent generalized density matrix method of Belyaev and Zelevinsky is analyzed. This deficiency appears as soon as one attempts to go beyond the semiclassical approximation equivalent to time dependent Hartree-Fock theory. A new version based on a revised factorization of the generalized two-body density matrix in terms of generalized one-body matrices is proposed. This factorization fulfills the requirements of antisymmetry and Hermiticity imposed by the properties of the exact two-body density matrix. It leads to a set of equations of motion which satisfy the conservation laws associated with the exact equations and guarantees that an energy-weighted and an energy-squared-weighted sum rule are fulfilled. Several associated approximate variational principles are described. The generalized-Hartree-Fock dynamics is salvaged in a reinterpretation as a generalized core-particle coupling model. Both the old and new theories coincide in the semiclassical limit where, in equivalent versions, they yield the time dependent Hartree-Fock and a self-consistent cranking theory. Standard applications to the random phase approximation are reviewed. Theories of damping of single-particle excitations and of random phase approximation phonons are proposed. The latter, in particular, carries the analysis to the point of including quantum corrections which differ in the new and old generalized density matrix theories, and thus pinpoint the need for the revised formulation.

I. INTRODUCTION

In 1962, A. Kerman and the author introduced a new method into the theory of nuclear collective motion, which we termed the generalized Hartree-Fock approximation[1-3] (GHFA). (Major aspects of this work, both foundations and subsequent applications, have been reviewed recently, both briefly[4,5] and at considerable length.[6]) A most important turn in the theoretical development resulted from the work of Marumori, Yamamura, and their collaborators[7,8] and the more extensive continuing development by Belyaev and Zelevinsky.[9,10] (A related approach by Mikhailov, Nadjakov, and their collaborators should be mentioned,[11-14] but will not be relevant to the discussion in this paper. Their work is reviewed briefly in Ref. 6.)

Despite the physically appealing character of the theoretical elements which enter in the formulation of the method(s) and the at least limited success of the applications not only to nuclear physics,[6] but also to condensed matter physics[15] and to quantum theories with soliton solutions,[16,17] it is fair to say that the practice of this method of studying band structure has more the air of a recondite art than of a widely accepted religion. This is perhaps reflected in the fact that the most recent theoretical monograph on nuclear collective motion[18] contains no systematic account of either the GHFA or of its alternative, the Belyaev and Zelevinsky generalized density matrix (GDM) method. This omission reflects the opinion in some quarters[19] that the methods are incomplete, inconsistent, or both.

One does not have to seek far to discover the reasons for this opinion. Several papers emanating from Munich some time ago,[20,21] which undertook a reexamination of the foundations of the subject, raised some justifiable questions. Unfortunately none of the interesting suggestions for improvement made in these papers was developed. Some time later, a series of papers by Friederich and collaborators[22-24] raised similar objections and provided some elements of a solution (to which we have since come by independent reasoning). Aside from the difference in the mode of reasoning, this work missed, inexplicably, an essential element of a complete formulation, namely the method of normalizing solutions based on the Pauli principle constraints, and thus it was not possible to carry out any nontrivial applications.

Unfortunately also for the public perception of our efforts, the writer has, for some time, been in disagreement with Belyaev and Zelevinsky concerning the precise form which the normalization condition should take. This difference is discussed later in this Introduction.

Before attempting to explain the basis for the present paper, an essential distinction should be drawn between two levels at which the ideas of our method can be implemented. At the first level, we start with a "fundamental" many-body Hamiltonian which contains the kinetic energy and some interaction which fits few-body data, and we then derive as much of the classical nuclear theory as possible. A somewhat less ambitious but certainly more realistic version of this same program would use an effective interaction of Skyrme-type in order to avoid the Brueckner part of this problem. It is toward the Skyrme-type of approach to this problem that the present work is primarily directed.

The fundamental dynamical problem, as always, is to find suitable approximations for many-body correlation functions in terms of a specified set of few-body (at most two-body) correlation functions. Prior to our initial work[1,2] this problem was always posed in terms of ground state correlations or of thermal averages. We widened the dialogue by suggesting that one contemplate simultaneously correlation functions defined over a set of collective states. The entire theoretical difficulty of the formulation consists in trying to choose a suitable approximate factorization formula. The major reason that this paper has been written is to improve on the previous formulations in this precise regard.

There is a second class of problems for which previous formulations may be less seriously flawed. This is the class in which one starts with a shell model Hamiltonian and tries to derive collective behavior. For schematic models in which the dynamics can be studied in relatively small vector spaces which span one or a few irreducible representations of a familiar Lie algebra, the fundamental decomposition problem is trivially solved by the completeness formula

$$\langle A \mid XY \mid B \rangle = \sum_C \langle A \mid X \mid C \rangle \langle C \mid Y \mid B \rangle \ , \tag{1.1}$$

where in the simplest case X and Y are generators of the Lie algebra and $\mid A \rangle$, $\mid B \rangle$, and $\mid C \rangle$ are all states in an irreducible representation. (In fact it suffices for either X or Y to be a generator.) Another simple case arises when X and Y is the component of a tensor of low rank under the interesting Lie algebra or can be well approximated by such an object. Such a situation arises physically when a realistic interaction is modeled by a sum of separable interactions (specificity forces) as in the well-known pairing plus quadrupole-quadrupole model. If we insist, however, on treating the shell model with residual forces of greater generality, we are back to some of the same difficulties as for a fundamental Hamiltonian, and the solution to be proposed will come into play.

Though we shall repeat matters in more detail in the body of the paper, let us summarize the essential elements from which all else flows, first as understood heretofore and then as modified in this paper. Let $\psi_a^\dagger$ (ψ_a) be creation (annihilation) operators for nucleons with single particle designation a, where either $a=(\vec{r},\sigma,\tau)$ represents space, spin, and isospin variables or $a=(n,l,j_a,m_a,\tau)$ are the usual spherical shell model set. Omitting pairing correlations, we study the equations of motion for the density operators

$$\hat{\rho}_{ab} = \psi_b^\dagger \psi_a \ , \tag{1.2}$$

and, in particular, try to confine our attention to a chosen subspace of "collective states" $\mid A \rangle$ (also designated as $\mid B \rangle$, $\mid C \rangle$, etc.) as described by the generalized matrix

$$\rho(aA \mid bB) \equiv \langle B \mid \psi_b^\dagger \psi_a \mid A \rangle \ . \tag{1.3}$$

Contemplation of the Heisenberg equation of motion for the object (1.3) shows us, in the usual way, that it is coupled to the two-body density matrix

$$\rho(abA \mid cdB) = \langle B \mid \psi_c^\dagger \psi_d^\dagger \psi_b \psi_a \mid A \rangle \ . \tag{1.4}$$

To *derive* the GDM equation of motion used by Belyaev and Zelevinsky[9,10] for a general interaction we must factorize (1.4) by the expression (summarion convention for intermediate states),

$$\rho(abA \mid cdB) \cong \langle B \mid \psi_c^\dagger \psi_a \mid C \rangle \langle C \mid \psi_d^\dagger \psi_b \mid A \rangle - (a \rightarrow b) \ . \tag{1.5}$$

This is the same factorization as we have used in our first paper,[1] where basically the same equation of motion is quoted in an appendix. However, our derivation of the equation is different. Instead of studying (1.3) directly, in our earliest work we studied a set of coefficients of fractional parentage

$$\Psi_i(aA) \equiv \langle i \mid \psi_a \mid A \rangle \ , \tag{1.6}$$

where $\mid i \rangle$ is some set of core-hole states having parentage in the collective set $\mid A \rangle$. In studying the equation of motion for (1.6), one is led, in place of (1.4) and (1.5), to consider the quantity

$$\langle i \mid \psi_c^\dagger \psi_b \psi_a \mid A \rangle \cong \langle i \mid \psi_a \mid B \rangle \langle B \mid \psi_c^\dagger \psi_b \mid A \rangle - (a \leftrightarrow b) \ , \tag{1.7}$$

where the factorization utilized for this case is shown.

As remarked correctly by Belyaev and Zelevinsky, (1.5) and (1.7) are distinct assumptions and none of their beautiful work (as summarized by Zelevinsky[10]) requires use of the equation of motion following from (1.7). It should be pointed out with equal justice, however, that the GHFA equation which results from the assumption (1.7) is a *solution* of their GDM equation in which $\rho(aA \mid bB)$, Eq. (1.3), is expressed as

$$\rho(aA \mid bB) = \sum_i \Psi_i(aA) \Psi_i^*(bB) \ , \tag{1.8}$$

i.e., the GDM equation follows from the GHFA equation under the assumption (1.8). Thus whatever the relative technical merits of each program, GHFA and GDM *dynamics* are, up to now, theoretically equivalent.

How about kinematics? If, in (1.5), one sets $b=c$ and notes that

$$\hat{N} \mid A \rangle = \sum_b \psi_b^\dagger \psi_b \mid A \rangle = N \mid A \rangle \ , \tag{1.9}$$

where N is the nucleon number, and thus

$$\hat{N} \psi_a \mid A \rangle = (N-1) \psi_a \mid A \rangle \ , \tag{1.10}$$

a straightforward consequence is the matrix equation

$$\rho^2 = \rho \ , \tag{1.11a}$$

i.e.,

$$\rho(aA \mid cC) \rho(cC \mid bB) = \rho(aA \mid bB) \ . \tag{1.11b}$$

In the past we have argued against the use of (1.11) on the grounds that in certain exactly soluble models, where the exact consequences of the Pauli principle have been worked out,[25,26] (1.11) gives the correct result only in the semiclassical limit equivalent to time dependent Hartree-Fock theory (TDHF) and that it is in error in the next order in Ω^{-1}, where Ω is the appropriate large parameter

characterizing the collective motion. This point has been both acknowledged and rebutted[10,27] with the remark that we should in any event restrict our attention to many body problems where Ω^{-1} is small.

It should now be clear that we have been *inconsistent* in our attitude in the past. On the one hand we have been happy to utilize the consequences of (1.5) for the dynamics, and on the other we have sought to reject it for the kinematics. The inescapable conclusion is that for general Hamiltonians (group theoretical models are exempted because of the way they are studied) the GDM and/or GHFA methods contain errors beyond the leading semiclassical limit.

As a special example of this problem, it turns out that the GDM equations of motion respect the conservation laws associated with the underlying Hamiltonian only to the semiclassical order. It was this particular realization that stimulated the present reconsideration.

The major "advance" of this paper is the replacement of (1.5) by the factorization

$$\rho(abA \mid cdB)=\tfrac{1}{2}[\langle B \mid \psi_c^\dagger \psi_a \mid C\rangle\langle C \mid \psi_d^\dagger \psi_b \mid A\rangle - (a\leftrightarrow b)-(c\leftrightarrow d)+(a\leftrightarrow b, c\leftrightarrow d)] . \tag{1.12}$$

In contrast to (1.5), this factorization satisfies all antisymmetry and Hermiticity requirements of $\rho(abA \mid cdB)$ and results, as we shall develop in the text, in a new GDM dynamics with all the desirable formal and limiting properties of the old GDM formulation. In addition it is conserving.

The factorization (1.12) was first proposed in print by Kamlah and Meyer,[20] but rejected on rather tenuous grounds. It was later resuscitated by Friedrich and collaborators,[22–24] but the need for kinematical constraints to provide normalization conditions was overlooked and therefore the scheme consisting basically only of the correct dynamics could not be implemented.

In Sec. II we formulate the dynamics and kinematics which follow from (1.12). The justification provided for this factorization shows that there is further room for improvement. [The residuum omitted in (1.12) will be the focus of future studies.] Nevertheless, as will be indicated from Secs. V on, the ansatz (1.12) is sufficiently rich to permit reasonable study of particle-hole excitations as well as damping of these excitations in closed shell nuclei. In Sec. II we also describe two different variational principles from which the dynamics follows.

In Sec. III, we reevaluate, in the light of the results of Sec. II, the relationship between GHFA and the old GDM dynamics. We find that though we have rejected the old GDM dynamics, it is not necessary to reject the GHFA dynamics. It is only necessary to require the *general form* (1.8) to go over a larger set of states than those which are described by GHFA dynamics; the latter then becomes a sophisticated core-particle coupling method.[28] It is no longer possible to derive old GDM dynamics from the core-particle equations and thus a possible source of inconsistency is removed.

In Sec. IV, we present the proof that the new GDM dynamics is conserving. The discussion includes a critical review of assertions[10] that the old GDM dynamics is also conserving. We maintain that there is a distinction between a conserving approximation and an accurate approximation, though both are desirable attributes. Replacing an exact expression by an approximate one is a one-way arrow, not to be reversed in any subsequent theoretical argument. The question of conservation is one concerning the structure of the *approximate* theory. A proof cannot include the reversal of the above arrow. With this understanding, old GDM dynamics is conserving either on the average or in the semiclassical limit, but not exactly. In Sec. IV, we also remark that there is a well-defined sense in which two sum rules are preserved, the energy-weighted and energy-squared-weighted rules.

In Sec. V, we study the semiclassical limit of the theory by means of the Wigner transform (WT) technique applied to the collective variables and thereby derive time-dependent Hartree-Fock theory and self-consistent cranking theory. Associated variational principles are presented. It is suggested that a possible basis for the Landau-Migdal theory is at hand.

In Sec. VI, we review elementary applications to vibrations and rotations. The latter case is important for understanding in what sense the WT technique can be applied to cyclic variables.

In Sec. VII, we describe a possible theory of damping of one-particle excitations implied by the GHFA dynamics. A standard description of such damping emerges.

Finally in Sec. VIII we outline the elements of a theory of damping of random-phase approximation (RPA) excitations. We explore the connection with previous work and convince ourselves that the new GDM dynamics is required to obtain that connection in a believable way. The old GDM equations omit essential "diagrams" in direct consequences of the differences that ensue from substitution of the incorrect factorization (1.5) for the "correct" factorization (1.12).

Four appendices are devoted to questions of supplemental and tangential interest.

II. DERIVATION OF NEW GENERALIZED DENSITY MATRIX EQUATIONS: VARIATIONAL PRINCIPLES

A. The equations of motion

We study a Hamiltonian of the form

$$H=h_{ab}\psi_a^\dagger\psi_b+\tfrac{1}{4}V_{abcd}\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c , \tag{2.1}$$

where we use summation convention wherever possible and the indices $a,b,\ldots,$ on the nucleon creation ($\psi^\dagger$), and annihilation (ψ) operators may refer either to space, spin, and isospin, $a=(\vec{r},\sigma,\tau)$, or may be the quantum numbers specifying a single-particle orbit. We take h and V to be Hermitian matrices

$$h_{ab}=h_{ba}^* , \tag{2.2}$$

$$V_{abcd}=V_{cdab}^* , \tag{2.3}$$

and V to describe the antisymmetrized matrix elements of a short range interaction,

$$V_{abcd} = -V_{bacd} = -V_{abdc} \ . \tag{2.4}$$

We suppose furthermore that H describes systems obeying Galilean relativity, namely that H commutes with the total momentum and total angular momentum operations and that V is Galilean invariant. We shall return to these points when we investigate whether the fundamental approximation proposed in this section is "conserving."[29]

In this first go around, we shall omit pairing correlations. Thus the specific formulation developed will be aimed at the study of the nuclear problem at closed shells. We start with dymamics by considering the equation of motion for the density operator

$$\hat{\rho}_{ab} = \psi_b^\dagger \psi_a \ , \tag{2.5}$$

$$[\hat{\rho}_{ab}, H] = h_{ac}\hat{\rho}_{cb} - \hat{\rho}_{ac}h_{cb} + \tfrac{1}{2}V_{acde}\psi_b^\dagger\psi_c^\dagger\psi_e\psi_d - \tfrac{1}{2}V_{cdbe}\psi_c^\dagger\psi_d^\dagger\psi_e\psi_a \ . \tag{2.6}$$

We are interested in the properties of a relatively small but experimentally prominent set of states—the collective states—including at the closed shells the ground state and the giant resonances. The members of the included set $| A \rangle$ are presumed to be eigenstates of H,

$$H | A \rangle = E_A | A \rangle \ . \tag{2.7}$$

In practice, assuming some optimum set of single particle states has been or will be established, the space of states $| A \rangle$ will be considered to be synonymous with the space of 0-particle, 0-hole (0p-0h) and 1p-1h states, or more ambitiously, will also include the 2p-2h space. The main point of our thrust is that we shall require a certain kind of mathematical and physical closure property in this space which will underlie all subsequent developments.

To bring this point to the fore, let us study the equation of motion for the generalized single-particle density matrix

$$\rho(aA \mid bB) = \langle B | \psi_b^\dagger \psi_a | A \rangle \ . \tag{2.8}$$

Then from (2.6) and (2.7) we calculate

$$(E_A - E_B)\rho(aA \mid bB) = h_{ac}\rho(cA \mid bB) - \rho(aA \mid cB)h_{cb} + \tfrac{1}{2}V_{acde}\rho(deA \mid bcB) - \tfrac{1}{2}V_{cdbe}\rho(aeA \mid cdB) \ , \tag{2.9}$$

and thus face the standard task of producing a closure approximation for the generalized two-body density matrix $\rho(abA \mid cdB)$,

$$\begin{aligned}\rho(abA \mid cdB) &\equiv \langle B | \psi_c^\dagger\psi_d^\dagger\psi_b\psi_a | A \rangle \\ &= -\rho(baA \mid cdB) \\ &= -\rho(abA \mid dcB) \\ &= \rho(cdB \mid abA)^* \ .\end{aligned} \tag{2.10}$$

We shall require of any closure approximation that it satisfy the antisymmetry and Hermiticity properties expressed in (2.10). This appears to be a minimum requirement, and therefore there is some obligation to explain why we[1,2] and others[9,10] who have approached the problem of collective motion through the equations of motion have nevertheless espoused approximations which fail to satisfy all the requirements of (2.10). This will be done in Sec. III. (In the Introduction we explained what was done, not why.)

An approximation which satisfies (2.10) was given in (1.12), namely,

$$\langle B | \psi_c^\dagger\psi_d^\dagger\psi_b\psi_a | A \rangle \cong \tfrac{1}{2}(\langle B | \psi_c^\dagger\psi_a | C \rangle\langle C | \psi_d^\dagger\psi_b | A \rangle - \langle B | \psi_c^\dagger\psi_b | C \rangle\langle C | \psi_d^\dagger\psi_a | A \rangle - \langle B | \psi_d^\dagger\psi_a | C \rangle\langle C | \psi_c^\dagger\psi_b | A \rangle + \langle B | \psi_d^\dagger\psi_b | C \rangle\langle C | \psi_c^\dagger\psi_a | A \rangle) \ . \tag{2.11}$$

Let us first record the consequences of this assumption and then return to consider its possible basis in fact. We substitute (2.11) in (2.9) and define both a collective Hamiltonian $\mathscr{H}_c$ with the matrix elements

$$\mathscr{H}_c(aA \mid bB) = \delta_{ab}\delta_{AB}E_A \ , \tag{2.12}$$

and a generalized Hartree-Fock Hamiltonian $\mathscr{H}$, with the matrix elements

$$\mathscr{H}(aA \mid bB) = h_{ab}\delta_{AB} + v(aA \mid bB) \ , \tag{2.13}$$

$$v(aA \mid bB) = V_{acbd}\rho(dA \mid cB) \ . \tag{2.14}$$

We then find that (2.9) takes the form of a matrix equation in the particle-collective labels (a,A), namely

$$[\mathscr{H}_c, \rho] = \tfrac{1}{2}[\mathscr{H}, \rho] + \tfrac{1}{2}[\mathscr{H}, \rho]_e \ , \tag{2.15}$$

where $(\mathscr{H}\rho)_e$ is a special matrix product defined by the expression

$$(\mathscr{H}\rho)_e(aA \mid bB) = \mathscr{H}(aC \mid cB)\rho(cA \mid bC) \ , \tag{2.16}$$

which involves an exchange of positions of the collective coordinates compared to the standard matrix product. If we replace the time-independent operators ψ_a by time dependent operators

$$\psi_a(t) = \exp(iHt)\psi_a\exp(-iHt) \ ,$$

we may replace (2.15) by the time-dependent equation

$$i\frac{d}{dt}\rho = \tfrac{1}{2}[\mathscr{H}, \rho] + \tfrac{1}{2}[\mathscr{H}, \rho]_e \ . \tag{2.17}$$

The unusual looking Eqs. (2.15) or (2.17) are accompanied by an equally unfamiliar generalization of the condition $\rho^2 = \rho$ described in conjunction with Eq. (1.11). If in Eq. (2.11) we set $b = d$, sum over b, and remember the conditions

$$\hat{N} | A \rangle = N | A \rangle \ , \tag{2.18}$$

$$\hat{N}\psi_a \mid A\rangle = (N-1)\psi_a \mid A\rangle \ , \tag{2.19}$$

where $\hat{N}$ is the number operator

$$\hat{N} = \psi_a^\dagger \psi_a \ , \tag{2.20}$$

and N is the number of nucleons in the state $\mid A\rangle$, we derive the condition[30]

$$\rho = \tfrac{1}{2}\rho^2 + \tfrac{1}{2}(\rho^2)_e \ . \tag{2.21}$$

Though this "derivation" is the natural generalization of one which works in the Hartree-Fock limit, the result (2.21) is suspect because there is a cancellation of the dominant terms and therefore (2.21) makes more extreme demands of the factorization (2.11) than are made by its use within the equations of motion. Nevertheless we shall base our theory on (2.15) and (2.21), reminding the reader that this requires that only *two* averages of (2.11) be accurate, no further demands being made on this factorization.

Equations (2.15) and (2.21) are major, but not sole elements of the proposed method. The Lie algebra satisfied by the density operators provides additional relationships which may be called into service in actual applications. This proposed additional element requires no special attention at the moment, however.

B. Derivation of factorization condition

We turn to the study of the basis for Eq. (2.11). As a first step in the derivation, we write identically, using the anticommutation relations

$$\langle B \mid \psi_c^\dagger \psi_d^\dagger \psi_b \psi_a \mid A\rangle = \tfrac{1}{2}(\langle B \mid \psi_c^\dagger \psi_a \psi_d^\dagger \psi_b \mid A\rangle - \delta_{ad}\langle B \mid \psi_c^\dagger \psi_b \mid A\rangle + \langle B \mid \psi_d^\dagger \psi_b \psi_c^\dagger \psi_a \mid A\rangle - \delta_{cb}\langle B \mid \psi_d^\dagger \psi_a \mid A\rangle) \ . \tag{2.22}$$

The purpose of this decomposition is the following: The first two terms of (2.22) are by themselves fully antisymmetric as are the last two terms. However, it suffices to provide approximations to the sum of the first two terms which are antisymmetric in a and b only, since the corresponding approximation for terms three and four will guarantee complete antisymmetry. The Hermiticity requirement will also be satisfied since the latter is separately satisfied between terms one and three and terms two and four.

Let us now write for the first two terms of (2.22),

$$\langle B \mid \psi_c^\dagger \psi_a \psi_d^\dagger \psi_b \mid A\rangle - \delta_{ad}\langle B \mid \psi_c^\dagger \psi_b \mid A\rangle = \langle B \mid \psi_c^\dagger \psi_a \mid C\rangle\langle C \mid \psi_d^\dagger \psi_b \mid A\rangle + [\langle B \mid \psi_c^\dagger \psi_a (1-P)\psi_d^\dagger \psi_b \mid A\rangle - \delta_{ad}\langle B \mid \psi_c^\dagger \psi_b \mid A\rangle] \ . \tag{2.23}$$

Here the sum on C is over the "collective" subspace and P is the projection operator for this space. Now the term in square brackets, involving a sum over intermediate states outside the collective subspace, *must* contain a part which provides the contribution necessary for antisymmetry. Where we have definite examples, this antisymmetrization arises from the *simplest* set of states omitted from the initial sum. Thus if the set $\mid A\rangle$ comprises only the ground state as in the Hartree-Fock factorization, then the antisymmetrization arises from one-particle, one-hole intermediate states.[31] If this well-known example generalizes,[15] the implication is that by antisymmetrizing we can obtain an approximate completeness or closure within a smaller subspace *than* if we employed a straightforward sum over intermediate states. The success of the closure depends on the choice of a suitable initial set $\mid A\rangle$. If we assume that by a suitable choice of this set the only effect of the terms in square brackets is to provide this antisymmetrization, then together with similar reasoning about the third and fourth terms of Eq. (2.22), we arrive at (2.11). Of course this cannot be exact, and we must eventually consider the errors involved. (The obvious omissions such as pairing and even Brueckner correlations can be included with relative ease as will be shown in subsequent work.)

There remain questions of more immediate concern in regard to our approximation:

(i) We have *a priori* no firm criteria for choosing the set $\mid A\rangle$ so that (2.11) is an optimal approximation. Our strategy here, as in the past, will be to explore the physical consequences of various attractive choices. Here we expect to go beyond previous applications, which to a large extent were either glorified versions of TDHF or else dealt more rigorously with schematic models.

(ii) We must consider the possibility of adding to (2.11) terms linear in the density matrix, e.g., a sum which is a multiple of

$$\delta_{ab}\langle B \mid \psi_c^\dagger \psi_b \mid A\rangle - \delta_{ac}\langle B \mid \psi_d^\dagger \psi_b \mid A\rangle - \delta_{bd}\langle B \mid \psi_c^\dagger \psi_a \mid A\rangle + \delta_{bc}\langle B \mid \psi_d^\dagger \psi_a \mid A\rangle \ . \tag{2.24}$$

We exclude such terms because they would contribute to a modification of (2.21) which would then not have the correct semiclassical limit, where (2.21) must reduce to the Hartree-Fock condition $\rho^2 = \rho$.

(iii) We shall emphasize later in this work that our approximation has two extremely attractive features—it reduces in the semiclassical limit to TDHF, and it is conserving. Previous efforts have had the first of these two properties, but only the present work also has the latter.

(iv) Since previous formulations have had associated variational principles of a rather attractive physical character, we have also sought a variational principle in the present case. We have found two, to be described later, one of which bears a resemblance to the work of Balian and Veneroni.[32,33] Neither, however, bears a resemblance to the "trace variational principle" which underlies the previous work. This seems somewhat surprising because of our previous investigations[34] which showed that such a principle underlies a formally exact version of Heisenberg

matrix mechanics. Therefore in Appendix A, we show that there is such a formally exact version in the present instance as well. It is probably not a useful approach to the present class of problems because too large a configuration space is needed to obtain convergence in sums over intermediate states.

It was precisely to reduce this problem to manageable size that we have introduced maximum antisymmetrization. On the other hand, we have become convinced that the solutions of Eqs. (2.15) and (2.21) do not minimize the trace of the Hamiltonian. We have two reasons for this conviction. First the variational principles associated with (2.15) are equivalent to a trace form only if we ignore the difference between the ordinary matrix product and the exchange matrix product defined in (2.16). Under these circumstances the formulation reduces to the previous ones and the variational principle given in the following can be transformed into the one previously known. The second reason is that an approximate trace form guarantees conservation laws only on average, whereas the consequences of (2.15) are stronger, as proved in Sec. IV.

C. Variational principle: First form

Consider the set of functionals

$$I_{ab}[\hat{Q}]=\mathrm{Tr}_c\hat{Q}\{[\hat{\rho}_{ab},\hat{H}]-i\dot{\hat{\rho}}_{ab}\}\ , \tag{2.25}$$

where Tr_c means trace over the chosen collective space $|A\rangle$, and Q is a member of a selected class of single-particle operators (collective operators) whose "in-band" matrix elements $\langle A|\hat{Q}|B\rangle$ are assumed to far exceed any interband elements. Thus we can evaluate

$$\begin{aligned}I_{ab}&\cong\langle A|\hat{Q}|B\rangle\langle B|\{[\hat{\rho}_{ab},\hat{H}]-i\dot{\hat{\rho}}_{ab}\}|A\rangle\\&\cong Q(B|A)\{\tfrac{1}{2}[\mathscr{H},\rho]+\tfrac{1}{2}[\mathscr{H},\rho]_e-[\mathscr{H}_c,\rho]\}(aA|bB)\\&=\mathrm{Tr}_cQ\{\tfrac{1}{2}[\mathscr{H},\rho]_{ab}+\tfrac{1}{2}[\mathscr{H},\rho]_{e,ab}-[\mathscr{H}_c,\rho_{ab}]\}\ .\end{aligned} \tag{2.26}$$

This evaluation "succeeds" because the assumed property of $\hat{Q}$ in confining the first intermediate sum allows us to employ the reasoning leading to (2.15). Therefore the condition

$$\delta I_{ab}\,/\delta Q(A|B)=0 \tag{2.27}$$

yields (2.15) *provided* we keep $\rho(aA|bB)$ fixed.

If we approximate (2.15) and (2.21) by the equations of the old GDM theory, i.e.,

$$[\rho,(\mathscr{H}-\mathscr{H}_c)]=\rho^2-\rho\cong 0\ , \tag{2.28}$$

then in place of (2.26), we have

$$I_{ab}^{\mathrm{approx}}=\mathrm{Tr}_cQ\{[\mathscr{H},\rho]_{ab}-[\mathscr{H}_c,\rho_{ab}]\}\ , \tag{2.29}$$

which can be written upon variation of the full trace

$$0=\sum_a\delta I_{aa}^{\mathrm{approx}}=\mathrm{Tr}\{[\rho,\delta Q](\mathscr{H}-\mathscr{H}_c)\}\ . \tag{2.30}$$

We observe next that any variation of the form

$$\delta\rho_{ab}=[\rho_{ab},\delta Q] \tag{2.31}$$

automatically satisfies the condition $\rho^2=\rho$ and

$$\mathrm{Tr}_c\mathscr{H}_{ab}\delta\rho_{ba}=\delta\,\mathrm{Tr}H\ , \tag{2.32}$$

where

$$\mathrm{Tr}H=h_{ab}\rho(bA|aA)+\tfrac{1}{2}v(aA|bB)\rho(bB|aA)\ . \tag{2.33}$$

We may consequently write

$$\sum_a\delta I_{aa}^{\mathrm{approx}}=\delta_\rho\mathrm{Tr}(H-\rho\mathscr{H}_c)=0\ , \tag{2.34}$$

where the usual symbol Tr means diagonal sum over single particle labels as well as over collective labels. Equation (2.34) is the variational principle of the old GDM dynamics. Here it is understood that $\delta\rho$ is properly constrained; otherwise the constraint has to be introduced with Lagrange multipliers.

D. Variational principle: Second form

The equations of motion (2.15) can also be recognized as the *solutions* of a more conventional variational condition, namely

$$\delta\langle A|H|A\rangle=0\ . \tag{2.35}$$

We restrict ourselves to variations of the form

$$\delta|A\rangle=\{i\epsilon_1(\hat{\rho}_{ab}\hat{Q}+\hat{Q}\hat{\rho}_{ab})+\epsilon_2[\hat{\rho}_{ab},\hat{Q}]\}|A\rangle\ , \tag{2.36}$$

where $\hat{Q}$ is again the class of collective one-particle operators considered in Sec. II C. From (2.35) and (2.36) we may conclude that

$$\begin{aligned}\langle A|[\hat{\rho}_{ab}\hat{Q},\hat{H}]|A\rangle&=0\\&=\langle A|\{[\hat{\rho}_{ab},\hat{H}]\hat{Q}+\hat{\rho}_{ab}[\hat{Q},\hat{H}]\}|A\rangle\ .\end{aligned} \tag{2.37}$$

The presence of the operator $\hat{Q}$, as in the previous considerations, is to keep sums over intermediate states confined to the collective space. In consequence, the commutators $[\hat{\rho}_{ab},\hat{H}]$ and $[\hat{Q},\hat{H}]$, where

$$\hat{Q}=q_{ab}\hat{\rho}_{ba}\ , \tag{2.38}$$

can be evaluated in the mode leading to (2.15). We thus obtain

$$\begin{aligned}0=\sum_{cd,B}q_{dc}\{&\rho(aB|bA)(\tfrac{1}{2}[\mathscr{H},\rho]+\tfrac{1}{2}[\mathscr{H},\rho]_e)(cA|dB)\\&+(\tfrac{1}{2}[\mathscr{H},\rho]+\tfrac{1}{2}[\mathscr{H},\rho]_e)\\&\times(aB|bA)\rho(cA|dB)\}\ .\end{aligned} \tag{2.39}$$

Having gone from the exact expression (2.37) to the approximate expression (2.39), its null value will nevertheless be guaranteed if the equation of motion (2.15) is satisfied, as one verifies immediately by substitution.

III. OLD GENERALIZED DENSITY MATRIX METHOD REVISITED

In this section we shall pinpoint and discuss the flaw in the previous work on this subject. It is appropriate to

start by studying the equations for single-particle coefficients of fractional parentage,

$$\Psi_i(aA)\equiv\langle i\mid\psi_a\mid A\rangle\ . \tag{3.1}$$

From the equations of motion

$$[\psi_a,H]=h_{ab}\psi_b+\tfrac{1}{2}V_{abcd}\psi_b^\dagger\psi_d\psi_c\ , \tag{3.2}$$

we can derive the equations

$$(E_A-E_i)\Psi_i(aA)=\mathscr{K}(aA\mid bB)\Psi_i(bB) \tag{3.3}$$

of the so-called generalized Hartree-Fock approximation (GHFA). The essential step leading to (3.3) is the factorization upon which much of our work has been based, namely,

$$\langle i\mid\psi_b^\dagger\psi_d\psi_c\mid A\rangle=\langle i\mid\psi_c\mid B\rangle\langle B\mid\psi_b^\dagger\psi_d\mid A\rangle-(c\leftrightarrow d)\ . \tag{3.4}$$

Notice that (3.4) asserts that there exists a set of states $\mid A\rangle$ of the even nucleus "N" and a corresponding set of states $\mid i\rangle$ of the $(N-1)$ nucleus such that the factorization (3.4) obtains.

In the early work, it was assumed that the set $\mid i\rangle$ exhausts the sum rule

$$\langle B\mid\psi_b^\dagger\psi_d\mid A\rangle=\rho(dA\mid bB)=\sum_i\Psi_i(dA)\Psi_i^*(bB)\ . \tag{3.5}$$

This would mean that (3.3) is genuinely a GHFA, since it would then be a nonlinear equation for the $\Psi_i(aA)$. We shall now show that this view is too naive. In fact, if (3.3) and (3.5) are both correct, it follows in an absolutely standard way that ρ itself satisfies the equation

$$[\mathscr{K}_c,\rho]=[\mathscr{K},\rho] \tag{3.6}$$

which contravenes Eq. (2.5). Does this mean that either (2.15) or (3.3) is wrong? Not necessarily, as we argue in the following.

The way out of the dilemma is to recognize that *given* the set $\mid A\rangle$, the set $\mid i\rangle$ for which (3.4) is justified (with $\mid B\rangle$ the *same* set as $\mid A\rangle$) is *smaller* than the set $\mid i\rangle$ needed to exhaust the sum rule (3.5). The general truth of this assertion can be seen from a simple example: consider a situation where $\mid A\rangle$ comprises the ground state and the one-phonon vibrational states. In Eq. (3.4) the set $\mid i\rangle$ must be restricted to one-hole and one-phonon, one-hole states. On the other hand, if $\mid A\rangle$ and $\mid B\rangle$ are one-phonon states in (3.5), we must expect two-phonon, one-hole states, which are not included in the GHFA in the approximation considered, to be as important as one-hole states for the sum considered (though neither is as important as one-phonon, one-hole states).

This does not imply that Eqs. (3.3) and the corresponding particle equation[1,2]

$$(E_p-E_A)\Phi_p(aA)=\mathscr{K}(aB\mid bA)\Phi_p(bB)\ , \tag{3.7}$$

where

$$\Phi_p(aA)\equiv\langle A\mid\psi_a\mid p\rangle\ , \tag{3.8}$$

are of no interest. Rather, except possibly for the special case of strongly decoupled sets of states, (3.3) is not to be viewed as defining a self-consistency problem, but rather one in which the eigenvalues E_A and the Hamiltonian $\mathscr{K}$ are given [having been determined from the solution of (2.15)], and thus (3.3) provides us with a *linear* problem. This point of view, when coupled with a semiphenomenological determination of the E_A and $\mathscr{K}$, has provided a most fruitful general formulation of the core-particle coupling method.[28,35–37]

In the past we have ignored the subtlety thrust upon us here. Though we have "always" been vaguely aware of its lurking dangers, we have chosen to ignore them precisely because of the attractive features of a true generalized Hartree-Fock approximation. Though both the old and the new version of the GDM method give back TDHF in the semiclassical limit, the need in future work to have a conserving approximation beyond that limit has finally commended the new approach over the old one.

IV. PROOF THAT THE APPROXIMATION IS CONSERVING AND SUM RULE PRESERVING

A. Conservation laws

The equation of motion (2.17) will be shown first to conserve momentum and angular momentum provided the fundamental Hamiltonian has this property. These two cases can be combined if we write the conditions for invariance in the form

$$(\theta_x+\theta_y)h_{xy}=0\ , \tag{4.1}$$

$$(\theta_x+\theta_y+\theta_z+\theta_w)V_{xyzw}=0\ , \tag{4.2}$$

where θ is the single particle momentum or angular momentum operator. We also assume that

$$\tilde{\theta}=-\theta\ , \tag{4.3}$$

where tilde represents transposed.

We wish to prove that

$$i\frac{d}{dt}\int dx\,\lim(x'\to x)\theta_x\rho(xA\mid x'A')=0\ . \tag{4.4}$$

Since the one particle term is conserving, we need only consider the interaction terms. For example, consider the *interaction* term from $[\mathscr{K},\rho]$ where by "integration by parts" and use of (4.3), we find as the contribution to (4.4)

$$\int\theta_xV_{xzyw}\rho(wA\mid zC)\rho(yC\mid xB)-\int\theta_x\rho(xA\mid yC)V_{yzxw}\rho(wC\mid zB)=\int(\theta_x+\theta_w)V_{xzyw}\rho(wA\mid zC)\rho(yC\mid xB)\ . \tag{4.5}$$

This would be the entire contribution of the interaction term if the time-dependent form of Eq. (3.6) was being considered. This approximation is not conserving (see the following). On the other hand, if we set $A=B$ and sum over the chosen space, then using the symmetry of the interaction, $V_{xzyw}=V_{zxwy}$, (4.5) *does* vanish. This is enough to ensure that the previous approximation is conserving *on the average*. More generally, Eq. (4.5) can be rewritten as

$$\frac{1}{2}\int(\theta_x+\theta_y+\theta_z+\theta_w)V_{xzyw}\rho(wA\mid zC)\rho(yC\mid xB)-\frac{1}{2}\int(\theta_y+\theta_z)V_{xzyw}[\rho(yA\mid xC)\rho(wC\mid zB)-\rho(wA\mid zC)\rho(yC\mid xB)]\ . \tag{4.6}$$

The first term vanishes, and we see that the nonvanishing term is a commutator in the collective space. As we shall see in more detail in Sec. V, this term vanishes in the semiclassical limit, which is the TDHF limit. (In fact in this limit the old and new GDM methods agree and are *both* conserving.)

Returning to the task at hand, we must calculate and add to (4.5) the contribution of the interaction term of $[\mathscr{H},\rho]_e$. By the same calculation as done for (4.5), it is easy to see that this term adds the missing piece to make up the first line of (4.6) (which vanishes) and nothing more. Thus our proof is complete.

We are also interested in number conservation. *All* the approximations considered thus far are number conserving. This follows from the property for this case, $\theta_x=1$, $\tilde{\theta}_x=\theta_x$. The proof for number conservation will become nontrivial when we add pairing correlations.

The proof that our approximation is conserving guarantees that spurious solutions of the equations of motion can be recognized by the fact that they occur at zero excitation energy. Of course this is not automatically guaranteed, but depends on defining properly orders of successive approximation. Superficially the matter is trivial in our case, since an examination of the proof just completed shows that cancellation occurs intermediate state by intermediate state.

There remains a point which requires further discussion. Belyaev and Zelevinsky aver that their version of GDM dynamics is conserving.[10] This appears to be in contradiction with our results. In the following we explain the basis for their conclusion which removes the formal mathematical discrepancy but still leaves a difference in point of view. The reconciliation, insofar as it is possible, arises from the changes or possible simplifications which can be introduced if one adheres to some version of the Copenhagen program of specificity forces, i.e., separable interactions.

Two philosophies toward the utilization of this program are possible here. In the first, we take no notice whatever of the suggested simplification until after we have derived from the theory developed in this paper all the dynamical and kinematical conditions of which we aim to make use. The effect of a general two-body interaction is then represented in our equations entirely in the form of generalized single particle potentials $v(aA\mid bB)$, which we are free to approximate in separable form (schematically written)

$$v(aA\mid bB)\cong\chi q^*_{ab}Q(A\mid B)\ , \tag{4.7}$$

or as a sum of such terms. This is our preferred point of view at the moment and one which we plan to exploit in the future.

In the more common approach we work from the beginning with a separable interaction which we write as

$$\tfrac{1}{2}\chi q^*_{ab}q_{cd}\psi^\dagger_a\psi^\dagger_c\psi_d\psi_b=U_{acbd}\psi^\dagger_a\psi^\dagger_c\psi_d\psi_b\ . \tag{4.8}$$

In place of Eq. (2.6) we have an equation in which $\frac{1}{2}V_{acde}\to U_{acde}$; because U_{acde} is separable, a different strategy for deriving dynamics is pursued, based on the assumption that sum rules involving the operator $\hat{Q}=q_{ab}\psi^\dagger_b\psi_a$ are saturated within the collective band. In this case, we use the method of Appendix A, straight sum over intermediate states, and write

$$\begin{aligned}&\langle B\mid\psi^\dagger_b\psi^\dagger_c\psi_e\psi_d\mid A\rangle\\&\quad=\langle B\mid\psi^\dagger_b\psi_d\psi^\dagger_c\psi_e\mid A\rangle-\delta_{dc}\langle B\mid\psi^\dagger_d\psi_e\mid A\rangle\\&\quad\to\langle B\mid\psi^\dagger_b\psi_d\mid C\rangle\langle C\mid\psi^\dagger_c\psi_e\mid A\rangle-\delta_{dc}\langle B\mid\psi^\dagger_b\psi_e\mid A\rangle\ .\end{aligned} \tag{4.9}$$

This decomposition, which can be justified, if at all, only because of the averaging with U_{acde}, yields old GDM theory with an *additional* single particle term arising from the second term of (4.9) of the form

$$\delta h_{ab}=-\chi q^*_{ac}q_{cb}\ , \tag{4.10}$$

and with $v(aA\mid bB)$ of the form (4.7).

If one now investigates whether the conservation laws are satisfied, one learns that they are not unless one permits the arrow in (4.9) *to reverse sign;* this step changes the GDM equations back into a matrix element of the original equations of motion, which are conserving by construction. However, this procedure begs the question, since it mixes up two distinct problems, the one of constructing an accurate approximation and the other of constructing a conserving approximation. In short, the approximation proposed in this paper, which we hope and believe will be accurate, is conserving by virtue of its structure, whether accurate or not. Again all differences are quantum corrections whose significance will be greater in future applications than in past ones (as shown for example in Sec. VIII).

B. Sum rules

We demonstrate that in a special sense, to be defined, our theory satisfies not only the energy-weighted sum rule but also the energy-squared-weighted sum. Concerning the former, if F is an arbitrary one particle Hermitian operator,

$$\hat{F}=f_{ab}\hat{\rho}_{ba}=\mathrm{Tr}f\hat{\rho} \tag{4.11}$$

and

$$S_k(F)\equiv\langle 0\mid\hat{F}(H-E_0)^k\hat{F}\mid 0\rangle\ , \tag{4.12}$$

then for $k=1$ we have as usual the two exact forms

$$\begin{aligned}S_1(F)&=\sum\omega_A\mid f_{0A}\mid^2\\&=\tfrac{1}{2}\langle 0\mid[\hat{F},[H,\hat{F}]]\mid 0\rangle\ ,\end{aligned} \tag{4.13}$$

$$f_{0A}=\langle 0\mid\hat{F}\mid A\rangle\ . \tag{4.14}$$

It is often stated that the RPA and, even more impressively, the generalized equation of motion method of Rowe[38,39] satisfy the sum rule (4.13). In fact these are provisos or "rules of the game." In the comparison of the two sides of (4.13) one does not use the exact operator $\hat{F}$, Eq. (4.11), but rather one replaces $\hat{F}$ by a different approximate operator, which we may call a generalized RPA operator, which is constructed so as to give the same matrix elements f_{0A} as $\hat{F}$ itself when evaluated between approximate eigenstates $|0\rangle$ and $|A\rangle$. When this same approximate operator is used to evaluate the double commutator in (4.13), an identity emerges. The basic reason is that the identity results from an average over the equations of motion which in this method are ultimately tied to the ground state expectation value of special double commutators.

In our method, we deal with the original form (4.11) of F. The matrix elements f_{0A} are calculated as linear combinations of generalized density matrix elements. On the other hand, we never calculate double commutators, but only single commutators. Therefore our method of evaluating the second form of (4.13) is to study the structure

$$\tfrac{1}{2}f_{0A}\langle A|[H,\hat{F}]|0\rangle-\tfrac{1}{2}\langle 0|[H,\hat{F}]|A\rangle f_{A0}\,. \tag{4.15}$$

But in fact, according to our approximations,

$$\begin{aligned}\langle A|[H,\hat{F}]|0\rangle &= f_{dc}\{\tfrac{1}{2}[\rho,\mathscr{H}](c0|dA)\\ &\quad+\tfrac{1}{2}[\rho,\mathscr{H}]_e(c0|dA)\}\\ &= f_{dc}[\rho,\mathscr{H}_c](c0|dA)\\ &= \omega_A f^*_{0A}\,.\end{aligned} \tag{4.16}$$

Combined with a similar evaluation for the second term, we easily reach an identity.

If we accept this as a "proof" that our approach also satisfies the S_1 rule, we have a bonus, namely by the same method the S_2 rule is also satisfied. In this case, we have

$$\begin{aligned}S_2(F)&=\sum(\omega_A)^2|F^2_{0A}\\ &=\langle 0|[\hat{F},H][H,\hat{F}]|0\rangle\,.\end{aligned} \tag{4.17}$$

In this form, the application of (4.16) will obviously serve up an identity. Here again the identities are exhibited as suitable averages over the equations of motion.

V. SEMICLASSICAL APPROXIMATIONS: VARIATIONAL PRINCIPLES, TIME DEPENDENT HARTREE-FOCK THEORY, AND GENERALIZED CRANKING THEORY

A. Semiclassical limit

We first show in general terms that the new GDM method differs only in quantum corrections from the old GDM. We rewrite (2.51) in the form

$$[\mathscr{H}_c,\rho]=[\mathscr{H},\rho]+\Delta\,, \tag{5.1}$$

$$\Delta=\tfrac{1}{2}[\mathscr{H},\rho]_e-\tfrac{1}{2}[\mathscr{H},\rho]\,. \tag{5.2}$$

We also write

$$\Delta(aA|bB)\equiv(A|\Delta_{ab}|B)\,, \tag{5.3}$$

thus considering Δ_{ab} as a matrix in the external or collective space. We thus find straightforwardly

$$\Delta_{ab}=\tfrac{1}{2}[\rho_{ac},v_{cb}]+\tfrac{1}{2}[\rho_{cb},v_{ac}]\,. \tag{5.4}$$

To understand the import of this result, we remark that, all cases of physical interest for low energy collective motion are contained in the assumption that the set of states A can be put into correspondence with a set of n coupled oscillators

$$\begin{aligned}|A\rangle=|\nu_1,\ldots,\nu_n\rangle&=\int|x^1,\ldots,x^n\rangle dx^1,\ldots,dx^n\langle x^1,\ldots,x^n|\nu_1,\ldots,\nu_n\rangle\,.\\ &\equiv\int|\underline{x}\rangle d\underline{x}\langle\underline{x}|\underline{\nu}\rangle\,.\end{aligned} \tag{5.5}$$

Of course the x^i will be organized into tensors under the appropriate symmetry groups, but we need not take this explicitly into account in the present considerations. The matrix structure of (5.4) may therefore be studied in the space of states $|\underline{x}\rangle$, where the x^i are an appropriate set of collective coordinates.

However, it has been emphasized innumerable times that once collective coordinates have been introduced, then the concepts of semiclassical limit and collectivity are inseparable.[40] This means that the matrices ρ_{ab} and v_{ab} which occur in (5.4) are almost local,

$$\langle\underline{x}|\rho|\underline{x}'\rangle\cong\rho(\underline{x})\delta(\underline{x}-\underline{x}')+\cdots\,, \tag{5.6}$$

where the missing terms (see the following) involve derivatives of the δ functions. In the approximation (5.6), Δ_{ab} of Eq. (5.4) vanishes and is thus a quantum correction. Applying similar reasoning to (2.21), we find that it can be replaced in the semiclassical limit by the more familiar condition $\rho=\rho^2$.

B. The Wigner transform

A more systematic approach which leaves us with the option of treating the quantum corrections with greater care is to apply the Wigner transform (WT) to the collective coordinates.[41] We write for an operator A,

$$\begin{aligned}\langle\underline{x}|A|\underline{x}'\rangle&\equiv\langle\underline{X}+\tfrac{1}{2}\underline{y}|A|\underline{X}-\tfrac{1}{2}y\rangle\\ &\equiv\tilde{A}(\underline{X},\underline{y})\,,\end{aligned} \tag{5.7}$$

where $\tilde{A}$ is assumed to be a slowly varying function of the average coordinates $\underline{X}$ and a rapidly varying function of

the difference coordinates $\underline{y}$. The WT, $A(\underline{X},\underline{P})$ of $\tilde{A}(\underline{X},\underline{y})$ is the Fourier transform with respect to $\underline{y}$,

$$A(\underline{X},\underline{P})=\int \exp(i\underline{y}\cdot\underline{P})d\underline{y}\tilde{A}(\underline{X},\underline{y}) . \tag{5.8}$$

The most important formula needed for application is the convolution theorem. Let

$$\langle \underline{x} \mid C \mid \underline{x}' \rangle = \int \langle \underline{x} \mid A \mid \underline{x}'' \rangle dx'' \langle \underline{x}'' \mid B \mid \underline{x}' \rangle . \tag{5.9}$$

Then

$$C(\underline{X},\underline{P})=\sum_{q=0}^{\infty}\sum_{r=0}^{\infty}(\tfrac{1}{2})^{q+r}(i)^{q-r}\frac{1}{q!}\frac{1}{r!} \times A_{qr}(\underline{X},\underline{P})B_{rq}(\underline{X},\underline{P}) , \tag{5.10}$$

where, e.g.,

$$A_{qr}=(\partial^q/\partial X^{i1},\ldots,\partial X^{iq}) \times(\partial^r/\partial P_{j_1},\ldots,\partial P_{j_r})A(\underline{X},\underline{P}) . \tag{5.11}$$

Thus to first order, we have

$$C(\underline{X},\underline{P})=A(\underline{X},\underline{P})B(\underline{X},\underline{P}) +\tfrac{1}{2}i\sum_i\left[\frac{\partial A}{\partial X^i}\frac{\partial B}{\partial P_i}-\frac{\partial A}{\partial P_i}\frac{\partial B}{\partial X^i}\right]+\cdots . \tag{5.12}$$

As we have argued previously,[41] if the collective coordinates have been properly identified, successive terms in the expansion (5.10) involve successively higher powers of a small parameter. This will be taken for granted in the following discussion. The semiclassical limit of the GDM method is defined by computation of the WT of Eqs. (2.15) [or (2.17)] and (2.21) and retention of the leading nonvanishing term.

C. Semiclassical limit

Unless we are dealing with a commutator in the collective space, matrix products are replaced by ordinary products, as in (5.12). This occurs for every term of (2.21), which we consider first. Therefore (2.21) becomes

$$\rho_{ab}(\underline{X},\underline{P})=\rho_{ac}(\underline{X},\underline{P})\rho_{cb}(\underline{X},\underline{P}) \tag{5.13}$$

or

$$\rho=\rho^2 . \tag{5.14}$$

The conclusion is that ρ is the density matrix of a Slater determinant depending on $2n$ parameters X,P. From the dynamics we shall establish that these are classical canonical pairs. Turning to (2.15), the left-hand side (lhs) is indeed a commutator with respect to the collective coordinates, since $\mathscr{H}_c$ is a unit matrix in the single-particle space, and thus the second term of (5.12) becomes relevant. The right-hand side (rhs) is a commutator in the internal space. We therefore obtain in detail

$$i\sum_i\left[\frac{\partial\mathscr{H}_c}{\partial X^i}\frac{\partial\rho_{ab}}{\partial P_i}-\frac{\partial\mathscr{H}_c}{\partial P_i}\frac{\partial\rho_{ab}}{\partial X^i}\right]=\mathscr{H}_{ac}\rho_{cb}-\rho_{ac}\mathscr{H}_{cb} , \tag{5.15}$$

where on the left-hand side we have a Poisson bracket and on the right-hand side a commutator.

The elements in (5.15) have the following meaning: $\mathscr{H}_{ac}$ is the Hartree-Fock Hamiltonian constructed with the density matrix $\rho_{ab}(\underline{X},\underline{P})$,

$$\mathscr{H}_{ab}=h_{ab}+v_{ab} =h_{ab}+V_{acbd}\rho_{dc} . \tag{5.16}$$

The collective Hamiltonian $\mathscr{H}_c$ has undergone several transformations to reach its place in (5.15). It appeared in (2.12) as a diagonal matrix of energies E_A. In the transformation (5.12), it becomes a matrix $\langle \underline{x} \mid \mathscr{H}_c \mid \underline{x}' \rangle$. In practice, however, we shall restrict ourselves to "quasi-local" operators, i.e., operators which are polynomials of at most finite order in the momentum variables. Thus we assume that $\mathscr{H}_c$ can reproduce the eigenvalues E_A provided it has the form

$$\mathscr{H}_c(\underline{x},\underline{p})=E_0+\mathscr{V}(\underline{x})+\tfrac{1}{8}\{\underline{p}_i,\{p_j,\mathscr{K}^{ij}(x)\},\} +\frac{1}{4}\frac{1}{2^4}\{p_i,\{p_j,\{p_k,\{p_l,\mathscr{L}^{ijkl}(\underline{x})\}\}\}\} +\cdots . \tag{5.17}$$

The fully symmetrized form, where odd powers of p have been excluded by a standard assumption about behavior under time reversal, has the advantage that it leads to an irreducibly simple WT, namely $\mathscr{H}_c(\underline{X},\underline{P})$, which appears in (5.15), has the *exact* form

$$\mathscr{H}_c(\underline{X},\underline{P})=E_0+\mathscr{V}(\underline{X})+\tfrac{1}{2}P_iP_j\mathscr{K}^{ij}(\underline{X}) +\tfrac{1}{4}P_iP_jP_kP_l\mathscr{L}^{ijkl}(\underline{X})+\cdots . \tag{5.18}$$

Combining (5.15) with the semiclassical limit of (2.17) allows us to write altogether

$$\dot{\rho}_{ab}=[\mathscr{H}_c,\rho_{ab}]_{\mathrm{PB}}=-i[\mathscr{H},\rho]_{ab} , \tag{5.19}$$

in which we have exhibited both time-dependent Hartree-Fock theory (for the special class of models considered) and the classical Liouville equation for the elements of the density matrix, PB of course standing for Poisson bracket. This is sufficient to identify the $\underline{X},\underline{P}$ as canonical pairs and $\mathscr{H}_c$ as the associated classical Hamiltonian.

Equations (5.14), (5.18), and (5.19) summarize the basic elements (with pairing to be added) of almost all existing practical microscopic theories of collective motion, which deal with the collective subspace as a Hilbert space. Thus the theory of adiabatic collective motion has recently been derived from this starting point, using the form (5.18) with terms at most of order two in the momentum.[41] By expanding $\mathscr{V}(\underline{X})$, $\mathscr{K}^{ij}(\underline{X})$, $\mathscr{L}^{ijkl}(\underline{X}),\ldots$, a theory of anharmonic vibrations drops out just as easily, with the RPA as the lowest approximation. A discussion of this and other standard applications is given in Sec. VI.

Of course, mapping the collective space onto a boson

space hardly exhausts the interesting possibilities. An equally interesting class of problems in which almost everything remains to be done involves the mapping of the collective space onto representations of Lie algebras.

D. "Variational" principle

Equation (5.15) can be given a variational formulation. First we shall state the appropriate variational principle and then show how it can be related to a previous variational formulation of the *old* GDM method. Equation (5.15) follows from the requirement that the functional

$$\mathcal{F}[\rho]=\int dX\,dP[\mathcal{E}(\rho)+\mathrm{Tr}\dot{\rho}q] \tag{5.20}$$

be stationary under variations $\delta\rho$ of the single particle density matrix induced by variations of an arbitrary skew-Hermitian single-particle matrix $\hat{q}(X,P)$, according to the requirement

$$\delta\rho_{ab}=[\delta q,\rho]_{ab}\ . \tag{5.21}$$

Here $\hat{q}$ is of the form (4.11), and is viewed as a WT with respect to the collective coordinates. The significance of (5.21) is that $\delta\rho$ of this form automatically satisfies the condition

$$\delta(\rho^2-\rho)=0\ . \tag{5.22}$$

Furthermore $\mathcal{E}(\rho)$ is the Hartree-Fock functional

$$\mathcal{E}(\rho)=\mathrm{Tr}[h\rho+\tfrac{1}{2}v\rho] \tag{5.23}$$

(or its generalization to include density dependent forces), and

$$\dot{\rho}=[\mathcal{H}_c,\rho]_{\mathrm{PB}} \tag{5.24}$$

is understood to be independent of ρ itself.

In fact, we calculate, using the properties of the Tr operation

$$\delta\mathcal{F}=\int dX\,dP\mathrm{Tr}\{[\rho,\mathcal{H}]-i[\rho,\mathcal{H}_c]_{\mathrm{PB}}\}\delta q=0 \tag{5.25}$$

and since δq is arbitrary, (5.15) follows. The variational principle holds for every value of X and P, and thus the integration can be dropped.

Equation (5.20) can be "deduced" from a variational principle for the old GDM method. The stationary quantity is [cf. (2.34)]

$$F=\mathrm{Tr}(H-\rho\mathcal{H}_c)\ , \tag{5.26}$$

subject to the *constraint* $\rho^2=\rho$, where matrix products and the Tr operation are in the combined space (a,A) or $(a,\underline{x})$. Because of the formal resemblance of the constraint to that of TDHF, the condition (5.21) on the variations may again be utilized with a suitably generalized interpretation. We thus conclude

$$\delta F=\mathrm{Tr}\{[\rho,(\mathcal{H}-\mathcal{H}_c)]\delta q\}\ . \tag{5.27}$$

If we rewrite (5.27) in terms of WT quantities and keep the leading nonvanishing term $\delta F\to\delta\mathcal{F}$ of (5.25) from which the starting point (5.20) was inferred. Equation (5.20) also appears to be a special case of a variational principle proposed by Balian and Veneroni,[32] as previously remarked.

E. Cranking variational principle

Equation (5.15) can also be recognized as the density matrix form of the self-consistent cranking theory. Thus if we write

$$\rho_{ab}(\underline{X},\underline{P})=\sum_\nu \psi_\nu(a\mid\underline{XP})\psi_\nu^*(b\mid\underline{XP})\ , \tag{5.28}$$

then (5.15) will be satisfied if we choose the single-particle functions as solutions of the self-consistent cranking equation

$$\epsilon_\nu(\underline{XP})\psi_\nu(a\mid\underline{X},\underline{P})=\mathcal{H}_{ab}\psi_\nu(b\mid\underline{XP})-i[(\partial\mathcal{H}_c/\partial X^i)(\partial/\partial P_i)-(\partial\mathcal{H}_c/\partial P_i)(\partial/\partial X^i)]\psi_\nu(a\mid\underline{XP})\ , \tag{5.29}$$

since from (5.29) and its complex conjugate, we readily deduce (5.15). Equation (5.29) can be derived from the requirement that a functional $\mathcal{G}$ be stationary under variations of $\psi_\nu^*(a\mid\underline{XP})$, where

$$\begin{aligned}\mathcal{G}=\int d\underline{X}\,d\underline{P}\{&\mathcal{E}(\rho)-(\partial\mathcal{H}_c/\partial X^i)\sum_\nu\psi_\nu^*(a\mid\underline{XP})(i\partial/\partial P_i)\psi_\nu(a\mid\underline{XP})\\&+(\partial\mathcal{H}_c/\partial P_i)\sum_\nu\psi_\nu^*(a\mid\underline{XP})(i\partial/\partial X^i)\psi_\nu(a\mid\underline{XP})-\sum_\nu\epsilon_\nu\psi_\nu^*(a\mid\underline{X},\underline{P})\psi_\nu(a\mid\underline{X},\underline{P})\}\ .\end{aligned} \tag{5.30}$$

VI. ELEMENTARY APPLICATIONS

A. Random phase approximation: Landau theory

We start with the limiting case of small vibrations by taking $\mathcal{H}_c(\underline{X},\underline{P})$ in the form

$$\begin{aligned}\mathcal{H}_c(\underline{X},\underline{P})&=\sum_i[(P_i^2/2B_i)+\tfrac{1}{2}C_iX_i^2]\\&=\sum_i\omega_ia_i^*a_i\ ,\end{aligned} \tag{6.1}$$

where

$$X_i=(2\omega_iB_i)^{-1/2}(a_i+a_i^*)\ , \tag{6.2}$$

$$P_i=-\tfrac{1}{2}i(\omega_iB_i)^{1/2}(a_i-a_i^*)\ , \tag{6.3}$$

define the complex canonical pairs a_i, ia_i^*. To investigate the consequences of (5.15) we introduce an expansion for the density matrix,

$$\rho=\rho^{(0)}+\rho_i^*a_i+\rho_ia_i^*+\cdots\ , \tag{6.4}$$

and a corresponding expansion for

$$\mathscr{H}=\mathscr{H}^{(0)}+\mathscr{H}_i^{(1)*}a_i+\mathscr{H}_i^{(1)}a_i^*+\cdots\ . \tag{6.5}$$

Introducing (6.1), (6.4), and (6.5) into (5.15), we obtain to zero and first order in the a_i, a_i^*,

$$[\mathscr{H}^{(0)},\rho^{(0)}]=0\ , \tag{6.6}$$

$$\omega_i\rho_i=[\mathscr{H}^{(0)},\rho_i]+[\mathscr{H}_i^{(1)},\rho^{(0)}]\ , \tag{6.7}$$

and the complex conjugate of (6.7). Equation (6.6) is, of course, the equation for the average static field, and if we write out the nonvanishing components of (6.7) in the representation in which $\rho^{(0)}$ is diagonal, we find (p=particle, h=hole),

$$\omega_i\rho_i(ph)=(\epsilon_p-\epsilon_h)\rho_i(ph)+v_i(ph)\ , \tag{6.8a}$$

$$-\omega_i\rho_i(hp)=(\epsilon_p-\epsilon_h)\rho_i(hp)+v_i(hp)\ . \tag{6.8b}$$

These two equations take the standard RPA form with the identification

$$\rho_i(ph)=X_i(ph)\ , \tag{6.9a}$$

$$\rho_i(hp)=Y_i(ph)\ , \tag{6.9b}$$

and the expanded expression

$$v_i(ab)=V_{ah'bp'}X_i(p'h')+V_{ap'bh'}Y_i(p'h')\ . \tag{6.10}$$

We have so far couched our discussion within the framework of a standard two-body interaction. However, there is no difficulty in including many-body forces, and as a special case, density dependent two-body forces, as long as the dependence can be approximated by polynomial form. The special case of the extension of our GDM dynamics to include three-body forces is taken up in Appendix B. Under these circumstances some additional complication of structure is encountered in the full GDM dynamics, but in the semiclassical limit, we again have an equation of the form (5.15), a generalized Hartree-Fock functional $\mathscr{E}(\rho)$ associated with a variational principle (5.20), and consequences for small vibrations as expressed by Eqs. (6.6) and (6.7). The only alteration is in the definition of the ingredients, which are

$$\mathscr{H}_{ab}=\delta\mathscr{E}/\delta\rho_{ba} \tag{6.11}$$

and

$$V_{abcd}=\delta\mathscr{E}(\rho)/\delta\rho_{db}\delta\rho_{ca}=\delta\mathscr{H}_{bd}/\delta\rho_{ca}$$
$$=\delta\mathscr{H}_{ab}/\delta\rho_{db}\ . \tag{6.12}$$

The Hartree-Fock plus RPA framework with the generalized definitions (6.11) and (6.12) of the ingredients has been termed Landau or Landau-Migdal theory of nuclei.[42,43] We believe that the theory proposed in this paper and extensions of it which we expect to develop provide a reasonable foundation for this theory.

B. Adiabatic limit: Two-dimensional rotations

As a second simple example of the application of the semiclassical equation (5.15), we consider the problem of rotations about a fixed axis. We are immediately faced with a new problem. The introduction of the WT in Sec. V contains the implicit assumption that we were dealing with a Cartesian metric with volume element $dx^1,\ldots,dx^n$. The form of the collective Hamiltonian (5.17) was chosen to be Hermitian with respect to this metric. Starting with such a description, we shall want to carry out a general point transformation—an example is the transformation from laboratory to intrinsic coordinates in the study of deformed nuclei. It is not difficult to prove[44] that if the Jacobian of the transformation is absorbed into a new definition of the wave function, then the transformed collective Hamiltonian may once again be determined in the form (5.17). However, if the original coordinates were each defined over its entire real axis, the new coordinates will have a different range and will usually include also cyclic variables. Therefore the Wigner transform used to reach (5.15) is not strictly applicable.

Nevertheless a simple approach is available in the adiabatic limit which yields the same result without assuming explicitly that the WT is valid. We illustrate for the example of motion about a fixed axis, but the method applies in general. Let us assume therefore that the collective space $|A\rangle$ corresponds to a set of eigenstates $|I\rangle$, where I is the angular momentum about the fixed axis.[45] We transform to a continuous representation by means of the eigenfunctions of the rigid plane rotor

$$(\theta\,|\,I)=(2\pi)^{-1/2}\exp(iI\theta) \tag{6.13}$$

according to the equation

$$|\theta\rangle=\sum_I|I\rangle(I\,|\,\theta) \tag{6.14}$$

and its inverse. In the θ representation we expand the matrix of an operator K in powers of the momentum operator

$$(\theta\,|\,K\,|\,\theta')=\tilde{K}(\Theta,\zeta)$$
$$=K^{(0)}(\Theta)\delta(\zeta)-iK^{(1)}(\Theta)\delta'(\zeta)$$
$$+\tfrac{1}{2}(-i)^2K^{(2)}(\Theta)\delta''(\zeta)+\cdots\ , \tag{6.15}$$

where the prime is derivative with respect to ζ and

$$\Theta=\tfrac{1}{2}(\theta+\theta'),\quad \zeta=(\theta-\theta')\ . \tag{6.16}$$

The quasilocal expansion (6.15) has the same justification as provided for the introduction of the WT.

Using (6.15) it is a simple exercise to show that for a product KL, we have

$$(\theta\,|\,KL\,|\,\theta')=(KL)^{(0)}\delta(\zeta)-i(KL)^{(1)}\delta'(\zeta)$$
$$+\tfrac{1}{2}(-i)^2(KL)^{(2)}\delta''(\zeta)+\cdots\ , \tag{6.17}$$

where

$$KL^{(0)}=K^{(0)}(\Theta)L^{(0)}(\Theta)+\tfrac{1}{2}iK^{(0)'}L^{(1)}-\tfrac{1}{2}iK^{(1)}L^{(0)'}$$
$$+\tfrac{1}{8}i^2K^{(0)''}L^{(2)}+\tfrac{1}{8}i^2K^{(2)}L^{(0)''}$$
$$-\tfrac{1}{4}i^2K^{(1)'}L^{(1)'}\ , \tag{6.18}$$

$$(KL)^{(1)}=K^{(0)}L^{(1)}+K^{(1)}L^{(0)}+\tfrac{1}{2}iK^{(0)'}L^{(2)}$$
$$-\tfrac{1}{2}iK^{(2)}L^{(0)'}$$
$$+\tfrac{1}{2}iK^{(1)'}L^{(1)}-\tfrac{1}{2}iK^{(1)}L^{(1)'}\ , \tag{6.19}$$

$$(KL)^{(2)}=K^{(0)}L^{(2)}+K^{(2)}L^{(0)}+2K^{(1)}L^{(1)} . \tag{6.20}$$

Indeed, since all that is involved in this derivation are the properties of the asymptotic representation (6.15) which confine all calculations to the neighborhood of the origin of ζ, the fact that ζ is a cyclic variable plays no role in this particular calculation. In short, the same results can be derived more quickly by applying formulas (5.8)–(5.11) for the WT. Thus, if we introduce a formal WT

$$\begin{aligned} K(\theta,J)&=\int \exp(-i\zeta J)\tilde{K}(\theta,\zeta) \\ &=K^{(0)}(\theta)+K^{(1)}(\theta)J+\tfrac{1}{2}K^{(2)}(\theta)J^2 \\ &\quad+\cdots , \end{aligned} \tag{6.21}$$

formulas (6.18)–(6.20) follow from the series in J ($\equiv P$) of both sides of (5.10). As opposed to (5.15), (6.18)–(6.20) contain some quantum corrections, however.

We shall be content here with the simplest of applications, the semiclassical approximation for two-dimensional rotation. Thus we write

$$\mathscr{H}_c(J)=J^2/2\mathscr{I} , \tag{6.22}$$

$$\begin{aligned} \rho(\theta,J)&=\rho^{(0)}(\theta)+\rho^{(1)}(\theta)(J/\mathscr{I}) \\ &\quad+\tfrac{1}{2}\rho^{(2)}(\theta)(J/\mathscr{I})^2 , \end{aligned} \tag{6.23}$$

$$\begin{aligned} \mathscr{H}(\theta,J)&=\mathscr{H}^{(0)}(\theta)+\mathscr{H}^{(1)}(\theta)(J/\mathscr{I}) \\ &\quad+\tfrac{1}{2}\mathscr{H}^{(2)}(\theta)(J/\mathscr{I})^2 , \end{aligned} \tag{6.24}$$

where the form of (6.24) follows from (6.22) and (6.23). Expanding both sides of (5.15) in powers of J, we find the equations

$$0=[\mathscr{H}^{(0)}(\theta),\rho^{(0)}(\theta)] , \tag{6.25}$$

$$-i\frac{d\rho^{(0)}}{d\theta}(\theta)=[\mathscr{H}^{(0)}(\theta),\rho^{(1)}(\theta)]+[\mathscr{H}^{(1)}(\theta),\rho^{(0)}(\theta)] . \tag{6.26}$$

As will be evident imminently these equations can be solved for $\theta=0$ and the results for $\theta\neq 0$ obtained by a suitable kinematical operation (rotation).

To evaluate the lhs of (6.26), from the definition (6.15) we find

$$\begin{aligned} \rho^{(0)}(\Theta)&=\int d\zeta(\theta\,|\,\hat{\rho}\,|\,\theta') \\ &=\int d\zeta\langle\Theta-\tfrac{1}{2}\zeta\,|\,\hat{\rho}\,|\,\Theta+\tfrac{1}{2}\zeta\rangle . \end{aligned} \tag{6.27}$$

Similarly

$$\rho^{(1)}(\Theta)=-i\int d\zeta\,\zeta\langle\Theta-\tfrac{1}{2}\zeta\,|\,\hat{\rho}\,|\,\Theta+\tfrac{1}{2}\zeta\rangle . \tag{6.28}$$

Remembering that

$$|\,\theta\rangle=\exp(-i\hat{J}\theta)\,|\,0\rangle \tag{6.29}$$

and if

$$\hat{J}=j_{ab}\hat{\rho}_{ba} , \tag{6.30}$$

we have

$$[\hat{J},\hat{\rho}_{ab}]=[\hat{\rho},j]_{ab} . \tag{6.31}$$

It follows from (6.27) to (6.30) that

$$\left.\frac{d\rho^{(0)}(\Theta)}{d\Theta}\right|_{\Theta=0}=-i[j,\rho^{(0)}] . \tag{6.32}$$

Thus setting $\Theta=0$ in (6.25) and (6.26) the latter becomes ($\theta=0$ understood)

$$-[j,\rho^{(0)}]=[\mathscr{H}^{(0)},\rho^{(1)}]+[\mathscr{H}^{(1)},\rho^{(0)}] . \tag{6.33}$$

By writing out (6.33) in the representation in which $\rho^{(0)}$ is diagonal and with the definitions

$$-\rho^{(1)}(ph)=X(ph)=-\rho^{(1)}(hp)^* , \tag{6.34}$$

$$(X)_{ph}=\begin{bmatrix} X(ph) \\ X(ph)^* \end{bmatrix} , \tag{6.35}$$

$$(j)_{ph}=\begin{bmatrix} j(ph) \\ j(ph)^* \end{bmatrix} , \tag{6.36}$$

(6.33) may be seen to have the familiar form

$$\underline{MX}=\underline{j} , \tag{6.37}$$

where M is the conventional RPA matrix,

$$M_{ph,p'h'}=\begin{bmatrix} A_{ph,p'h'} & B_{ph,p'h'} \\ \tilde{B}_{ph,p'h'} & \tilde{A}_{ph,p'h'} \end{bmatrix} , \tag{6.38}$$

where

$$A_{ph,p'h'}=(\epsilon_p-\epsilon_h)\delta_{pp'}\delta_{hh'}+V_{ph',hp'} , \tag{6.39a}$$

$$B_{ph,p'h'}=V_{pp',hh'} , \tag{6.39b}$$

and the tilde implies transpose.

To complete this discussion we must check the self-consistency of the assumption (6.22), i.e., we must compute the moment of inertia. Alternatives for this computation include energy self-consistency

$$\langle I\,|\,\hat{H}\,|\,I\rangle=E_{I=0}+I^2/2\mathscr{I} , \tag{6.40}$$

generally applicable or, in the present case, the simpler alternative

$$\langle I\,|\,\hat{J}\,|\,I\rangle=I . \tag{6.41}$$

The computation of (6.41) will illustrate the transition from the semiclassical calculation leading to (6.37) back to quantum theory. Thus we have

$$\begin{aligned} I=\langle I\,|\,\hat{J}\,|\,I\rangle&=\int d\theta\,d\theta'(I\,|\,\theta)\langle\theta\,|\,\hat{J}\,|\,\theta'\rangle(\theta'\,|\,I) \\ &=\frac{1}{2\pi}\int d\zeta\,d\Theta\exp(-i\zeta I)\mathrm{Tr}j(\theta'\,|\,\rho\,|\,\theta) \\ &=\frac{1}{2\pi}\int d\Theta\,\mathrm{Tr}\rho^{(0)}(\Theta) \\ &\quad-(I/\mathscr{I})\int\frac{d\Theta}{2\pi}\mathrm{Tr}j\rho^{(1)}(\Theta) , \end{aligned} \tag{6.42}$$

where we have used Eq. (6.23), to first order. For consistency we must have

$$\frac{1}{2\pi}\int d\Theta \,\mathrm{Tr} j\rho^{(0)}(\Theta)=0\ , \tag{6.43}$$

$$\mathscr{I}=-\frac{1}{2\pi}\int \mathrm{Tr} j\rho^{(1)}(\Theta)\ . \tag{6.44}$$

We show that we may set $\Theta=0$ in the integrand of (6.43) and (6.44). We consider $\hat{\rho}$ in the original "circular" representation, $\hat{\rho}_{mm'}=\psi^{\dagger}_{m'}\psi_m$, and

$$\exp(i\hat{J}\theta)\psi^{\dagger}_m\exp(-i\hat{J}\theta)=\exp(im\theta)\psi^{\dagger}_m\ . \tag{6.45}$$

It follows from (6.27) or (6.28) that

$$\rho^{(i)}_{mm'}(\theta)=\exp[i(m'-m)\theta]\rho^{(i)}_{mm'}(0)\ . \tag{6.46}$$

Thus the angular averages reduce the conditions (6.43) and (6.44) to

$$\mathrm{Tr} j\rho^{(0)}=0\ , \tag{6.47}$$

$$\mathscr{I}=-\mathrm{Tr} j\rho^{(1)}=\mathrm{Tr} j^{\dagger}X\ , \tag{6.48}$$

where the definitions (6.34)—(6.36) have been recalled. (In two dimensions the nonvanishing matrix elements j_{ab} have $m_a=m_b$.) With $\rho^{(0)}$ chosen even under time reversal, (6.47) is satisfied, and (6.48) in conjunction with (6.37) yields the well-known self-consistent cranking moment of inertia.

A complete treatment of the adiabatic limit in the semiclassical limit by the methods of Wigner transform have been given in a separate publication to which the reader is referred.[41] For a serious treatment of quantum corrections, we must study the new GDM dynamics, a program which remains before us.

In concluding the discussion of the previous two sections, it is worthwhile emphasizing that although we have gone to the semiclassical limit, no "requantization" is necessary in our approach. The relation to a full quantum theory remains intact and can be invoked when necessary, as in (6.40) and (6.41).

VII. MODEL FOR SINGLE PARTICLE WIDTHS

In this section and, more particularly, in the next one, we outline calculations which take us at least one step beyond the semiclassical approximations. Here we consider a model for single particle widths and there a model for the widths of giant resonances. In this latter case the new GDM dynamics yields a different theory than the old one; indeed the observation of an obvious lack of exchange symmetry convinced the writer of the necessity of proposing the revisions discussed in this paper.

A theory of particle and hole widths follows from the structure of the GHFA. From our present point of view, however, we are instructed to follow a certain order in solving the equations of the theory. In particular we must start with (2.15) and (2.21).

A. GDM dynamics

We study (2.15) in the weak coupling approximation. In this approximation, which corresponds roughly to the limit of small oscillations, the matrix elements $\rho(aA\mid bB)$ can be classed into definite sets with respect to average numerical size if we first sort the states $\mid A\rangle$ into subsets:

$$\begin{aligned}&\mid 0\rangle \ \text{ground state}\ ,\\ &\mid A_1\rangle \ \text{1 phonon or 1p-1h space}\ ,\\ &\mid A_2\rangle \ \text{2 phonon or 2p-2h space}\ .\end{aligned} \tag{7.1}$$

Thus if Ω^{-1} is the characteristic small parameter of the model, where Ω will be the order of the number of particle-hole configurations, we assume the following hierarchy for elements needed in our subsequent discussion

$$\rho(aA\mid bA)=\text{elements diagonal in collective space}=0(1) \tag{7.2}$$

$$\rho(a\,0\mid bA_1)\sim\rho(aA_1\mid b\,0)\sim 0(\Omega^{-1/2})\ , \tag{7.3}$$

$$\rho(aA_1\mid bB_1)(B_1\neq A_1)\sim\rho(a\,0\mid bA_2)\sim\cdots\sim 0(\Omega^{-1})\ . \tag{7.4}$$

Of course these assumptions turn out to be self-consistent.

Thus in lowest order, we study the equation for

$$\rho(a\,0\mid b\,0)=\rho^{(0)}_{ab}\ , \tag{7.5}$$

which involves

$$\mathscr{H}(a\,0\mid b\,0)\cong\mathscr{H}^{(0)}_{ab}\ . \tag{7.6}$$

Together with the condition $\rho^{(0)}=(\rho^{(0)})^2$ rederived below, this defines Hartree-Fock theory. In the single-particle representation in which $\rho^{(0)}$ is diagonal, the labels h designate occupied orbitals and the labels p unoccupied orbitals.

We next consider the quantities (7.3), for which only the elements $(a,b)=(p,h)$ or (h,p) are nonvanishing (as is well-known and rederived again below). The linearized equations for the nonvanishing elements $\rho(a\,0\mid bA_1)$ and $\rho(aA_1\mid b\,0)$ are the RPA equations. These are the terms of $O(\Omega^{-1/2})$. In Sec. VIII, we shall be interested in the next order terms in the RPA equations, which are of $O(\Omega^{-3/2})$ and provide the damping mechanism for the RPA states. Therefore let us write out the appropriate equations to this order. By straightforward enumeration and rearrangement, we find that we can present the result in the form

$$\omega_A\rho(pA\mid h\,0)=(\epsilon_p-\epsilon_h)\rho(pA\mid h\,0)+v(pA\mid h\,0)+R_1+R_2+R_3\ , \tag{7.7}$$

plus the equation with $(p\leftrightarrow h)$. In displaying the correction terms R_1—R_3 in the following, the symbols A_1 and A_2 will have the meaning assigned to them in conjunction with (7.3) and (7.4), except that sums over A_1 exclude specifically the one-phonon state A under study. We then have

$$2R_1(pA\mid h0)=v(pA\mid p'A_1)\rho(p'A_1\mid h0)-\rho(pA\mid bA_1)v(bA_1\mid h0)+v(pA_1\mid b0)\rho(bA\mid hA_1)$$
$$-\rho(pA_1\mid h'0)v(h'A\mid hA_1)\,, \tag{7.8}$$

which describes transitions within the one-phonon space. In the Copenhagen model,[46] these are the main terms which contribute to the width. We also have

$$2R_2=v(pA\mid bA_2)\rho(bA_2\mid h0)-\rho(pA\mid h'A_2)v(h'A_2\mid h0)+v(pA_2\mid p'0)\rho(p'A\mid hA_2)$$
$$-\rho(pA_2\mid b0)v(bA\mid hA_2)\,, \tag{7.9}$$

which describes the excitation of two phonon states or 2p-2h states. The decay of a high-lying phonon into two low-lying ones is a mode possibly competitive with the mode described by R_1, though the present evidence[46] is that the terms of the latter dominate. Finally, the term R_3, which has the form

$$2R_3=v(pA\mid h'0)[\rho(h'0\mid h0)-\delta_{h'h}]+[v(pA\mid p'A)-\delta_{pp'}v_p]\rho(p'A\mid h0)$$
$$-\rho(pA\mid p'A)v(p'A\mid h0)+\rho(pA\mid h'0)[v(h'0\mid h0)-v_h\delta_{hh'}]$$
$$+[v(p0\mid p'0)-v_p\delta_{pp'}]\rho(p'A\mid h0)+v(pA\mid h'0)[\rho(h'A\mid hA)-\delta_{hh'}]$$
$$-\rho(pA\mid h'0)[v(h'A\mid hA)-v_h\delta_{hh'}]-\rho(p0\mid p'0)v(p'A\mid h0)\,, \tag{7.10}$$

describes corrections to the Hartree-Fock description of the ground state (ground state correlations) as well as blocking corrections. A few such terms are studied in Appendix C.

The quantity $\rho(pA\mid h0)$ is the Tamm-Dancoff or shell model amplitude of the state $\mid A\rangle$. The corresponding equation for the ground state correlation amplitude $\rho(hA\mid p0)$ is obtained by the interchange $(p\leftrightarrow h)$, $(p'\leftrightarrow h')$ in (7.7)–(7.10). In this section we require only the standard RPA approximation as input to the further study below.

B. GDM kinematics

We next explore (2.21) and related matters. Without presenting any details, it is straightforward to derive the standard conditions in order unity and order $\Omega^{-1/2}$, which describe, respectively, the determinantal character of $\rho(a0\mid b0)$ and the vanishing of the p-p and h-h elements of $\rho(aA\mid b0)$ and $\rho(a0\mid bA)$. To find higher order corrections—the ground state correlations for instance—we have found it more convenient in the past to switch to a different method of calculation, the so-called number operator method.[47,48] Since we do not propose to carry out a serious investigation of these corrections in this paper, we shall not pursue this matter further here. A brief account of the technique applied is provided in Appendix C.

C. GHFA dynamics

We suppose that the HF and RPA problems have been solved at a level where even the escape width of RPA states arising from continuum single particle states has been included.[49,50] We next fold in the GHFA dynamics for particle states. Defining

$$\Phi_p(aA)=\langle A\mid\psi_a\mid p\rangle \tag{7.11}$$

by studying its equation of motion and using the factorization

$$\langle A\mid\psi_a^\dagger\psi_b\psi_c\mid p\rangle=\langle A\mid\psi_a^\dagger\psi_b\mid B\rangle\langle B\mid\psi_c\mid p\rangle-(b\leftrightarrow c)\,, \tag{7.12}$$

we derive the equation

$$(\mathscr{E}_p-\omega_A)\Phi_p(aA)=\mathscr{H}(aB\mid bA)\Phi_p(bB)\,, \tag{7.13}$$

where

$$\mathscr{E}_p=E_p-E_0 \tag{7.14}$$

and $\omega_A=E_A-E_0$ as usual.

We wish to investigate the spreading width for the states $\mid p\rangle$ implied by Eq. (7.13). Here we take $\mid A\rangle\rightarrow\mid 0\rangle$. In working out the rhs of (7.13), we encounter the term

$$\mathscr{H}(a0\mid b0)\Phi_p(b0)=\epsilon_a\Phi_p(a0)$$
$$+[v(a0\mid b0)-\delta_{ab}v_a]\Phi_p(b0)\,. \tag{7.15}$$

Retaining only the term $b=a$ on the rhs (see the following), we have approximately

$$\mathscr{H}(a0\mid b0)\Phi_p(b0)\cong(\epsilon_a+\delta\epsilon_a)\Phi_p(a0)\,, \tag{7.16}$$

where (Appendix C)

$$\delta\epsilon_a\cong\tfrac{1}{2}\sum_{ph,A}\mid Y_{ph}(A)\mid^2[V_{apap}-V_{ahah}]\,. \tag{7.17}$$

Similarly we shall write

$$\mathscr{H}(aA\mid bA)\Phi_p(bA)\cong[\epsilon_a+\delta\epsilon_a(A)]\Phi_p(aA)\,, \tag{7.18}$$

where (Appendix C)

$$\delta\epsilon_a(A)\cong\delta\epsilon_a+\sum_{ph}[\mid Y_{ph}(A)\mid^2+\mid X_{ph}(A)\mid^2]$$
$$\times[V_{apap}-V_{ahah}]\,. \tag{7.19}$$

With these approximations, we consider the pair of equations for $\Phi_p(a0)$ and $\Phi_p(aA)$ in which we include the coupling of the first amplitude to the second and the

second back to the first and ignore the coupling of the one-phonon states to higher sectors. The equations of interest are

$$[\mathscr{E}_p-(\epsilon_a+\delta\epsilon_a)]\Phi_p(a0)=\sum_{bA} v(aA\mid b0)\Phi_p(bA)\ , \tag{7.20}$$

$$\{\mathscr{E}_p-\omega_A-[\epsilon_b+\delta\epsilon_b(A)]\}\Phi_p(bA) = \sum_c v(b0)\mid cA)\Phi_p(c0)\ . \tag{7.21}$$

Following the standard procedure, we solve (7.21) for $\Phi_p(bA)$ and substitute in (7.20). Since some of the ϵ_b will be continuum energies and some of the ω_A as well, the solution of (7.21) becomes well-defined only if we replace $\mathscr{E}_p$ by $\mathscr{E}_p+\frac{1}{2}i\Delta$, where Δ can be viewed either as an interval for energy averaging or as average width for the sum $\omega_A+(\epsilon_a+\delta\epsilon_a)$ which the latter acquires in consequence of the coupling of the associated states to higher sectors. With definitions $\bar{\epsilon}_a=\epsilon_a+\delta\epsilon_a$ and $\bar{\epsilon}_a(A)=\epsilon_a+\delta\epsilon_a(A)$, we obtain finally

$$\left\{(\mathscr{E}_p-\epsilon_a)\delta_{ac} - \sum_{bA}\frac{v(aA\mid b0)v(b0\mid cA)}{[\mathscr{E}_p-\frac{1}{2}i\Delta-\omega_A-\bar{\epsilon}_b(A)]}\right\}\Phi_p(c0)=0\ . \tag{7.22}$$

In Eq. (7.22), a, b, and c are all particle states where a and c must carry the same j value as p and a is identified with p in the limit of no coupling. If we ignore contributions from modes $c\neq a$ we obtain a dispersion relation of standard structure for determination of ϵ_p, namely,

$$0=\mathscr{E}_p-\bar{\epsilon}_p+\sum_{p'A}\frac{|v(pA\mid p'0)|^2}{\mathscr{E}_p-\omega_A-\bar{\epsilon}_{p'}(A)+\frac{1}{2}i\Delta}\ . \tag{7.23}$$

This formula differs in detail from the expression obtained by formal partial summation of Feynman diagrams,[51] though there is agreement if one compares the most significant contributions, numerically, to the width, namely the forward going graphs.

If we write

$$\mathscr{E}_p=\bar{\epsilon}_p+\Delta\mathscr{E}_p-\tfrac{1}{2}i\Gamma_p\ , \tag{7.24}$$

$$\mathscr{E}_{Ap'}=\omega_A+\bar{\epsilon}_{p'}(A)\ , \tag{7.25}$$

we have

$$\Delta\mathscr{E}_p=\sum_{p'A}\frac{|v(pA\mid p'0)|^2(\mathscr{E}_p-\mathscr{E}_{Ap'})}{(\mathscr{E}_p-\mathscr{E}_{Ap'})^2+\frac{1}{4}\Delta^2}\ , \tag{7.26}$$

$$\Gamma_p=\Delta\sum_{p'A}\frac{|v(pA\mid p'0)|^2}{(\mathscr{E}_p-\mathscr{E}_{Ap'})^2+\frac{1}{4}\Delta^2}\ . \tag{7.27}$$

To evaluate these expressions, according to our philosophy, we can at this point introduce specificity forces in the guise of schematic values for the matrix elements. The resulting expressions, which will not be developed here, resemble in structure those evaluated by the Copenhagen group.[46,51]

Equation (7.23) may also be written

$$G^{-1}(\mathscr{E}_p)=0\ , \tag{7.28}$$

where $G(z)$ is our approximation to the one-particle Green's function. This point is amplified in Appendix D, and allows us to compute the strength function following the well-known method also reviewed there.

VIII. MODEL FOR DAMPING OF RPA EXCITATIONS

In Eq. (7.7) we have grouped correction terms to the RPA into three sets $R_i(pA\mid h0)$, $i=1,2,3$. The last term R_3 exhibited in Eq. (7.10), describes real shifts in the single particle and single-hole energies. These terms will not be analyzed further in this paper. The terms R_2 given in (7.9) describe the vertex for the phonon A to turn into a p-h pair through a two-phonon intermediate state. Here we shall refer to the quantity $v(pA\mid h0)$ as a vertex function and $\rho(pA\mid h0)$ as an amplitude. In Fig. 1, which represents the terms of R_2, and in succeeding figures, a vertex will be represented by a triangle, an amplitude by a circle. It is possible for energy conserving intermediate states to occur in some of the contributions if the two phonons are low energy ones. Within the present formalism such terms are more complicated and probably less significant than the class contain in R_1, and they will therefore not be dealt with in detail here.

The simplest model for damping appears to be hidden in this latter set of terms. We can obtain insight into the structure of these terms from Fig. 2. Not all the terms arising from Fig. 2 give rise to energy-conserving intermediate states; we shall see later how to settle this point.

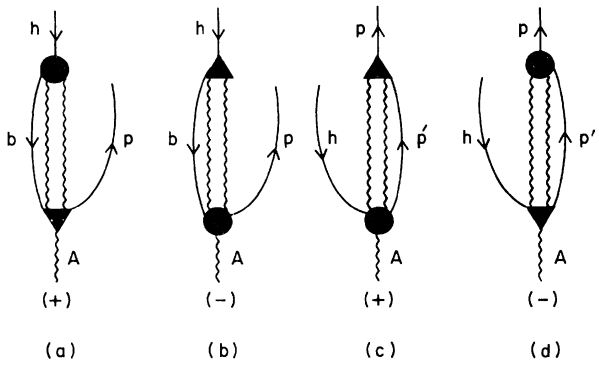

FIG. 1. Diagrammatic representation of the terms in $R_2(pA\mid h0)$, defined in Eq. (7.9). Here solid lines represent particles or holes according to the labeling. Both types of lines may occur with either sense for the arrow; this sense determines the sign of the corresponding contribution to an energy denominator. Wavy lines describe phonons. A full triangle with various incoming and outgoing lines stands for a generalized single-particle potential v, also called a vertex; a full circle with similar attachments is associated with an amplitude ρ. The overall sign of the term, for which a rule is developed in the text, appears below the diagram.

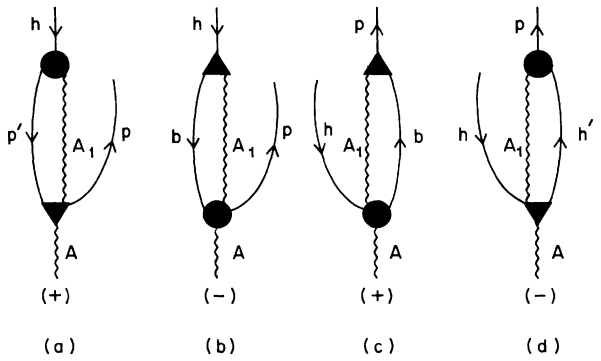

FIG. 2. Diagrammatic representation of the terms in $R_1(pA \mid h0)$, defined in Eq. (7.8). The elements are as in Fig. 1.

One unusual property of these diagrams is that arrows on particle and hole lines can have either sense with respect to the "flow of time," which can be taken as upwards. This sense determines the sign with which the energy of the particle occurs in an energy denominator.

We have no intention in this preliminary discussion of presenting a full analysis of $R_1(pA \mid h0)$. We want to make a few specific points which we consider most germane for highlighting the structure of the contributions. Toward this end, we study the terms

$$2R_{11}(pA \mid h0) \equiv -\rho(pA \mid h'A_1)v(h'A_1 \mid h0) + v(pA_1 \mid p'0)\rho(p'A \mid hA_1) . \tag{8.1}$$

Comparison with (7.8) shows that we have selected pieces of the second and third terms, i.e., pieces of Figs. 2(b) and 2(c) with $b=h'$ and $h=p'$, respectively. To evaluate (8.1), the next step is to obtain equations of motion for the amplitude $\rho(pA \mid h'A_1)$.

We present only the results of such an analysis whose main ingredient is the recognition of which intermediate states yield the contributions of dominant interest. Two kinds of contributions commend themselves. One contains elements such as[52]

$$\mathscr{H}(aA \mid bA) \cong \mathscr{H}(a0 \mid b0) \cong \epsilon_a \delta_{ab} \tag{8.2}$$

multiplying the amplitude under study. The other, which provides the driving terms, gives a product of an RPA amplitude and a vertex. The result is

$$[\omega_A - \epsilon_p - \omega_{A_1} + \epsilon_{h'}]\rho(pA \mid h'A_1) = \tfrac{1}{2}[v(pA \mid p'0)\rho(p'0 \mid h'A_1) + v(p0 \mid p'A_1)\rho(p'A \mid h'0) - \rho(pA \mid h''0)v(h''0 \mid h'A_1) - \rho(p0 \mid h''A_1)v(h''A \mid h'0)] . \tag{8.3}$$

Note that for an unstable state $\mid A\rangle$ and a continuum ϵ_p the square bracket on the lhs of (8.3) can vanish and thus the "solution" of (8.3) for $\rho(pA \mid h'A_1)$ requires introduction of the same device, $\omega_A \to \omega_A + i\frac{1}{2}\Delta$, as in Sec. VII. We shall *understand* that this has been done.

Before introducing (8.3) into (8.1), we shall make another simplification. It is time to remember that

$$\rho(pA \mid h0) = \rho(h0 \mid pA)^*$$

is a "forward going" or Tamm-Dancoff amplitude, whereas

$$\rho(p0 \mid hA) = \rho(hA \mid p0)^*$$

is a "backward going" or ground-state correlation amplitude. For simplicity of presentation, we shall omit the contributions from the latter. With this understanding, we obtain from (8.3) and (8.1),

$$\begin{aligned} 4R_{11}(pA \mid h0) = &- \sum [\omega_A - \omega_{A_1} - \epsilon_p + \epsilon_{h'}]^{-1}[v(p,0 \mid p'A_1)\rho(p'A \mid h'0)v(h'A_1 \mid h0) \\ &\quad - \rho(pA \mid h''0)v(h''0 \mid h'A_1)v(h'A_1 \mid h0)] \\ &+ \sum [\omega_A - \omega_{A'} - \epsilon_{p'} + \epsilon_h]^{-1}[v(pA_1 \mid p'0)v(p'0 \mid p''A_1)\rho(p''A \mid h0) \\ &\quad - v(pA_1 \mid p'0)\rho(p'A \mid h'0)v(h'0 \mid hA_1)] . \end{aligned} \tag{8.4}$$

The four terms displayed are represented by the four diagrams of Fig. 3, in the same order. The energy denominator is given in each case by the structure of the intermediate state with A_1 present as $\omega_A - \omega_{A'} - \underline{\epsilon}$ (upward-going line) $+$ ϵ (downward-going line). The overall sign of each term is easily traced to the commutator structure of the equations of motion, where factors $v\rho$ correspond to $(+)$, ρv to $(-)$, and this rule must be applied twice if there is one energy denominator.

We now remark: The contributions (8.4) and Fig. 3 are precisely the ones which underlie the damping theory of Bortignon and Broglia.[46,51,53] Since our theory is not tied

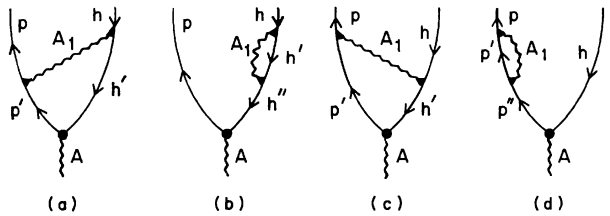

FIG. 3. A subset of the contributions to R_1, the terms in Eq. (8.1) of the text.

to specificity forces, we have the option for the further evaluation of using a fundamental interaction or of introducing a specificity (separable) assumption for the evaluation of the vertices v.

Before continuing, we note that the structure summarized in Fig. 3 is tied essentially to our use of the new dynamics. In the old dynamics, three of the terms would be missing and the fourth would be multiplied by four. We are truly dealing with quantum effects where the difference between the two forms of the dynamics is decisive.

We are interested in making only one additional observation in this brief discussion, namely that there are additional terms in $R_1(pA \mid h0)$ which can contribute to the damping. We shall consider but one example. In order to evaluate the first term of R_1, Eq. (7.8), we need to write an expanded form of the vertex,

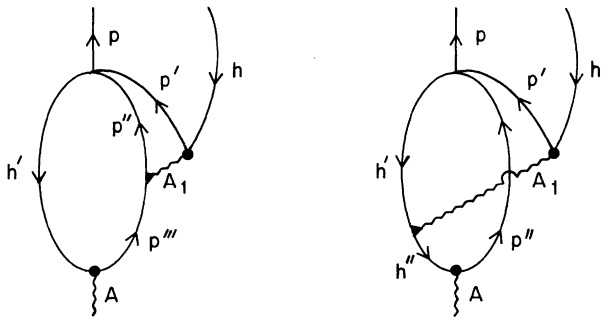

FIG. 4. Diagrams of contributions to R_1 given in Eq. (8.6), which may have energy conserving intermediate states and are distinct from those of Fig. 3. These diagrams each contain an explicit vertex of the interaction V, as opposed to previous diagrams where such factors are contained within the vertices v.

$$\begin{aligned} v(pA \mid p'A_1) = & V_{pp'''p'p''}\rho(p''A \mid p'''A_1) \\ & + V_{ph''p'h'}\rho(h'A \mid h''A_1) \\ & + V_{ph'p'p''}\rho(p''A \mid h'A_1) \\ & + V_{pp''p'h'}\rho(h'A \mid p''A_1)\,. \end{aligned} \tag{8.5}$$

The contribution of the third term of (8.5) to the first term of R_1 will be written with the help of (8.3) as

$$\begin{aligned} 4R_{12} = & \sum V_{ph'p'p''}[\omega_A - \omega_{A_1} - \epsilon_{p''} + \epsilon_{h'}]^{-1} \\ & \times [v(p''0 \mid p'''A_1)\rho(p'''A \mid h'0)\rho(p'A_1 \mid h0) - \rho(p''A \mid h''0)v(h''0 \mid h'A_1)\rho(p'A_1 \mid h0)]\,, \end{aligned} \tag{8.6}$$

and represented in Fig. 4. The energy denominators have the same structure (nature and relative signs of the single particle energy contributions) as those of Fig. 3 and can thus contribute to the width. This was the result we were after.

As with a number of other topics introduced in this paper, further work remains to be carried out.

IX. SUMMARY AND CONCLUSIONS

We have presented a new and, we believe, improved version of the GDM method which is based on a closure approximation in the equations of motion which, though suggested in part by previous authors, has either been subsequently rejected by them or incompletely implemented. We have emphasized that the new proposal has both dynamical and kinematical consequences. We have compared the new method with the previous GDM method and with the GHFA and pointed out that though the former is no longer fully tenable, the latter remains valid if reinterpreted as a core-particle coupling theory.

We have shown that the semiclassical limit of the new theory remains TDHF, the new and old theories differing only in quantum corrections beyond this limit. Most important, the new theory satisfies the conservation laws and several sum rules. We have furthermore explained why the claim that the old theory is conserving cannot be sustained in general.

Finally we outlined a theory of damping of single-particle and collective excitations. The discussion of the latter has been included in order to illustrate at least one important application where the difference in content between old and new GDM dynamics is decisive and the former yields obviously incorrect results.

This work was supported in part by the U.S. Department of Energy under Contract No. EY-76-C-02-3071.

APPENDIX A

We describe a formally exact version of the equations of motion with an attached variational principle. The equation of motion (2.9) can be written

$$\begin{aligned} (E_A - E_B)\rho(aA \mid bB) = & h_{ac}\rho(cA \mid bB) - \rho(aA \mid cB)h_{cb} \\ & + U_{acde}\rho(deA \mid bcB) \\ & - \rho(aeA \mid cdB)U_{cdbe}\,, \end{aligned} \tag{A1}$$

where U_{abcd} is the unsymmetrized matrix element of the interaction, namely

$$V_{abcd}=U_{abcd}-U_{bacd}$$
$$\equiv U_{badc}-U_{abdc}\ . \tag{A2}$$

To transform (A1) we utilize two different exact factorizations, namely for the third term of (A1) we write

$$\langle B\mid\psi_b^\dagger\psi_c^\dagger\psi_e\psi_d\mid A\rangle=\langle B\mid\psi_b^\dagger\psi_d\mid C\rangle\langle C\mid\psi_c^\dagger\psi_e\mid A\rangle$$
$$-\delta_{cd}\langle B\mid\psi_b^\dagger\psi_e\mid A\rangle\ , \tag{A3}$$

which requires a *complete* set of intermediate states. For the fourth term of (A1), we write instead

$$\langle B\mid\psi_c^\dagger\psi_d^\dagger\psi_e\psi_a\mid A\rangle=\langle B\mid\psi_d^\dagger\psi_e\mid C\rangle\langle C\mid\psi_c^\dagger\psi_a\mid B\rangle$$
$$-\delta_{ce}\langle B\mid\psi_d^\dagger\psi_a\mid A\rangle\ . \tag{A4}$$

With the help of (A3) and (A4), (A1) can be written in the form

$$[\mathscr{H}_c,\rho]=[\mathscr{K},\rho]\ , \tag{A5}$$

where $\mathscr{K}$ is an effective Hamiltonian,

$$\mathscr{K}(aA\mid bB)=\delta_{AB}\bar{h}_{ab}+u(aA\mid bB)\ , \tag{A6}$$

$$\bar{h}_{ab}=h_{ab}-U_{accb}\ , \tag{A7}$$

$$u(aA\mid bB)=U_{acbd}\rho(dA\mid cB)\ . \tag{A8}$$

Equations (A5)–(A8) are formally exact.

To obtain a variational principle, we need a constraint equation for the density ρ. To the identity

$$\langle B\mid\psi_b^\dagger\psi_c(\psi_e\psi_d+\psi_d\psi_e)\mid A\rangle=0\ . \tag{A9}$$

We apply the factorization (A3), set $c=e$ and sum over c. Using number conservation, we then derive the consequence

$$\rho^2-(\Omega-N+1)\rho=0\ , \tag{A10}$$

where N is the number of nucleons and Ω is the total number of single particle states, which we assume to be finite. As strange as it appears, (A10) is formally exact.

We turn then to the variational principle. Writing the Hamiltonian in the form

$$H=h_{ab}\psi_a^\dagger\psi_b+\tfrac{1}{2}U_{abcd}\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c \tag{A11}$$

and employing the factorization (A3) [(A4) gives the same result], we calculate

$$F\equiv\mathrm{Tr}H-\tfrac{1}{2}U_{accb}\rho(bA\mid aA)$$
$$=\mathrm{Tr}\mathscr{K}\rho-\tfrac{1}{2}\mathrm{Tr}u\rho$$
$$=\mathrm{Tr}(\bar{h}\rho+\tfrac{1}{2}u\rho)\ . \tag{A12}$$

This expression has the property

$$\delta F/\delta\rho(bB\mid aA)=\mathscr{K}(aA\mid bB)\ . \tag{A13}$$

Consequently if we define the functional G as

$$G=F-\mathrm{Tr}\mathscr{H}_c\rho-\mathrm{Tr}\Lambda[\rho^2-(\Omega-N+1)\rho]\ , \tag{A14}$$

where Λ is a Lagrange multiplier matrix, and require

$$\delta G/\delta\rho=0=\mathscr{K}-\mathscr{H}_c-\rho\Lambda-\Lambda\rho+(\Omega-N+1)\Lambda=0\ , \tag{A15}$$

the result can be viewed as an equation for Λ *provided* $\mathscr{H}_c$ and ρ (and therefore $\mathscr{K}$) are known. That $\mathscr{K}$ and $\mathscr{H}_c$ are as advertised is checked by proving that (A5) follows from (A15) provided that (A10) is satisfied. That this is true is verified by calculating

$$0=[\rho,\delta G/\delta\rho]\ . \tag{A16}$$

(A5) may also be derived directly from variation of $(F-\mathrm{Tr}\mathscr{H}_c\rho)$ provided $\delta\rho$ automatically satisfies (A10), as it does in the form analogous to (5.21), namely

$$\delta\underline{\rho}=[\underline{\rho},\delta D]\ . \tag{A17}$$

APPENDIX B

In this appendix, we consider the additional terms which occur in the GDM equation when we add three-body forces to the Hamiltonian of the form

$$\frac{1}{3}\frac{1}{3!}V_{abc,def}\psi_a^\dagger\psi_b^\dagger\psi_c^\dagger\psi_f\psi_e\psi_d\ , \tag{B1}$$

where

$$V_{abc,def}=V_{bac,edf}=\text{etc.} \tag{B2}$$

and

$$V_{abc,def}=-V_{bac,def}=V_{bca,def}=\text{etc.}, \tag{B3}$$

i.e., $V_{abc,def}$ is symmetric under comparable exchanges of the first three and the last three indices and has the appropriate sign under an odd or even permutation of either the first three or the last three indices.

In the equation of motion (2.6), let us replace the indices a,b by x,y, i.e., we study $[\hat{\rho}_{xy},H]$. The extra terms on the rhs of (2.6) are then

$$\frac{1}{3!}V_{xbc,def}\psi_y^\dagger\psi_b^\dagger\psi_c^\dagger\psi_f\psi_e\psi_d-\frac{1}{3!}V_{abc,dey}\psi_a^\dagger\psi_b^\dagger\psi_c^\dagger\psi_x\psi_e\psi_d\ . \tag{B4}$$

The appropriate generalization of the factorization (2.11) is conjectured to be

$$\langle A'\mid\psi_a^\dagger\psi_b^\dagger\psi_c^\dagger\psi_f\psi_e\psi_d\mid A'\rangle=\frac{1}{3!}\sum\epsilon_{i_1i_2i_3}\epsilon_{j_1j_2j_3}\langle A'\mid\psi_{i_1}^\dagger\psi_{j_1}\mid A''\rangle\langle A''\mid\psi_{i_2}^\dagger\psi_{j_2}\mid A''\rangle\langle A'''\mid\psi_{i_3}^\dagger\psi_{j_3}\mid A\rangle\ , \tag{B5}$$

where the sum runs separately over all permutations of *abc* and *def* and ϵ is the alternating symbol.

The sorting out of the contributions to the equations of motion is only slightly tedious. The result can be expressed in terms of a new generalized single particle potential which is a double matrix in the collective space, namely

$$U(sAA' \mid yA''A''') = V_{xbc,yde}\rho(dA \mid bA''')\rho(eA' \mid cA'') = U(xA'A \mid yA'''A'') . \quad \text{(B6)}$$

We define the matrix products

$$(U\rho)(xA \mid yA') = U(xAA''' \mid zA''A''')\rho(zA'' \mid yA') , \quad \text{(B7)}$$

$$(U\rho)_{e_1}(xA \mid yA') \equiv U(xA''A''' \mid zA''A')\rho(zA \mid yA''') , \quad \text{(B8)}$$

$$(U\rho)_{e_2}(xA \mid yA') = U(xAA'' \mid xA'A''')\rho(zA''' \mid yA'') . \quad \text{(B9)}$$

The additional contributions may then be written

$$\tfrac{1}{3}[U,\rho] + \tfrac{1}{3}[U,\rho]_{e_1} + \tfrac{1}{3}[U,\rho]_{e_2} . \quad \text{(B10)}$$

In the semiclassical limit, the three terms become equal.

APPENDIX C

We are interested in studying the effect of ground state correlations on restricted elements of the density matrix, namely $\rho(h0 \mid h0)$, $\rho(p0 \mid p0)$, $\rho(hA \mid hA)$, and $\rho(pA \mid pA)$. These are particularly required in Sec. VII in order to obtain the results reported in Eqs. (7.17) and (7.19). First of all consider

$$\rho(hA \mid hA) = \langle A \mid \psi_h^\dagger \psi_h \mid A \rangle . \quad \text{(C1)}$$

We reduce the calculation of this quantity to that of $\rho(h0 \mid h0)$ by using the quasiboson operators

$$Q^\dagger(A) = \sum_{ph} [X_{ph}(A)\psi_p^\dagger \psi_h - Y_{ph}(A)\psi_h^\dagger \psi_p] , \quad \text{(C2)}$$

where

$$X_{ph}(A) = \langle 0 \mid \psi_h^\dagger \psi_p \mid A \rangle = \rho(pA \mid h0) , \quad \text{(C3)}$$

$$Y_{ph}(A) = \rho(hA \mid p0) . \quad \text{(C4)}$$

We have

$$\mid A \rangle = Q^\dagger(A) \mid 0 \rangle , \quad \text{(C5)}$$

$$Q(A) \mid 0 \rangle = 0 , \quad \text{(C6)}$$

and

$$[Q(A), Q^\dagger(A)] \mid 0 \rangle = \mid 0 \rangle , \quad \text{(C7)}$$

but

$$\langle 0 \mid [Q(A), \psi_h^\dagger \psi_h] \mid A \rangle = -\sum_p [\mid X_{ph}(A) \mid^2 + \mid Y_{ph}(A) \mid^2] , \quad \text{(C8)}$$

where the last evaluation uses the correct fermion algebra. We thus find

$$\rho(hA \mid hA) = \rho(h0 \mid h0) - \sum_p [\mid X_{ph}(A) \mid^2 + \mid Y_{ph}(A) \mid^2] . \quad \text{(C9)}$$

Similarly we can show

$$\rho(pA \mid pA) = \rho(p0 \mid p0) + \sum_h [\mid X_{ph}(A) \mid^2 + \mid Y_{ph}(A) \mid^2] . \quad \text{(C10)}$$

Thus we have only to study

$$\rho(h0 \mid h0) = 1 - \langle 0 \mid \psi_h \psi_h^\dagger \mid 0 \rangle$$

and

$$\rho(p0 \mid p0) = \langle 0 \mid \psi_p^\dagger \psi_p \mid 0 \rangle .$$

For this purpose we utilize the "number operator method."[47,48] In this method we can replace the hole counting operator $\psi_h \psi_h^\dagger$ and the particle counting operator $\psi_p^\dagger \psi_p$ by expansions in particle hole creation and annihilation operators when acting on the ground state. We have

$$\psi_h \psi_h^\dagger \to \sum_p B_{ph}^\dagger B_{ph} - \tfrac{1}{2} \sum_{pp'h'} B_{ph}^\dagger B_{p'h'}^\dagger B_{p'h'} B_{ph} + \cdots , \quad \text{(C11)}$$

$$\psi_p^\dagger \psi_p \to \sum_h B_{ph}^\dagger B_{ph} - \tfrac{1}{2} \sum_{hp'h'} B_{ph}^\dagger B_{p'h'}^\dagger B_{p'h'} B_{ph} + \cdots , \quad \text{(C12)}$$

where

$$B_{ph}^\dagger = \psi_p^\dagger \psi_h = (B_{ph})^\dagger . \quad \text{(C13)}$$

Equations (C11) and (C12) are accurate up to the level of 2p-2h mixtures in the ground state, but representations of arbitrary accuracy can be given[48] and there are corresponding formulas for operators such as $\psi_h \psi_{h'}^\dagger$ and $\psi_p^\dagger \psi_{p'}$, i.e., hole and particle scattering operators.

For the evaluation of (C11) and (C12), we find

$$\langle 0 \mid B_{ph}^\dagger B_{ph} \mid 0 \rangle = \sum_A \langle 0 \mid B_{ph}^\dagger \mid A \rangle \langle A \mid B_{ph} \mid 0 \rangle = \sum_A \mid Y_{ph}(A) \mid^2 \quad \text{(C14)}$$

and

$$\sum_{p'h'} \langle 0 \mid B_{ph}^\dagger B_{p'h'}^\dagger B_{p'h'} B_{ph} \mid 0 \rangle = \sum_{p'h'} \langle 0 \mid B_{ph}^\dagger B_{p'h'}^\dagger \mid 0 \rangle \langle 0 \mid B_{p'h'} B_{ph} \mid 0 \rangle + 0(Y^4) = \sum_{AA'p'h'} Y_{ph}(A) X_{p'h'}^*(A) X_{p'h'}(A') Y_{ph}^*(A') \cong \sum_A \mid Y_{ph}(A) \mid^2 . \quad \text{(C15)}$$

In this evaluation, we have used the approximate RPA normalization

$$\sum_{ph}[X^*_{ph}(A)X_{ph}(A')-Y^*_{ph}(A)Y_{ph}(A')]$$
$$\cong\sum_{ph}X^*_{ph}(A)X_{ph}(A')=\delta_{AA'}\,. \quad \text{(C16)}$$

Thus to 2p-2h accuracy, we find

$$\langle 0\,|\,\psi_h\psi^\dagger_h\,|\,0\rangle=\tfrac{1}{2}\sum_{p,A}|\,Y_{ph}(A)\,|^2\,, \quad \text{(C17)}$$

$$\langle 0\,|\,\psi^\dagger_p\psi_p\,|\,0\rangle=\tfrac{1}{2}\sum_{h,A}|\,Y_{ph}(A)\,|^2\,. \quad \text{(C18)}$$

Finally we apply (C17), (C18), and afterwards (C9) and (C10) to the evaluation of shifts in single-particle energies. For instance

$$\delta\epsilon_a=v(a0\,|\,a0)-v_a$$
$$=-\sum_h V_{ahah}\langle 0\,|\,\psi_h\psi^\dagger_h\,|\,0\rangle+\sum_p V_{apap}\langle 0\,|\,\psi^\dagger_p\psi_p\,|\,0\rangle$$
$$\cong\tfrac{1}{2}\sum_{ph\,A}|\,Y_{ph}(A)\,|^2(V_{apap}-V_{ahah})\,. \quad \text{(C19)}$$

Similarly

$$\delta\epsilon_a(A)=v(aA\,|\,aA)-v_a$$
$$=\delta\epsilon_a+\sum_{ph}[\,|\,Y_{ph}(A)\,|^2+|\,X_{ph}(A)\,|^2]$$
$$\times(V_{apap}-V_{ahah})\,. \quad \text{(C20)}$$

These are the results quoted in Eqs. (7.17) and (7.19).

APPENDIX D

In terms of the matrix element studied in Sec. VII, the strength function for detecting the "single-particle" state $|p\rangle$ at energy E when a particle in the single-particle mode a is added to the ground state of the system is

$$P_a(E)=\sum_p|\,\Phi_p(a0)\,|^2\delta(E-\mathscr{E}_p)\,, \quad \text{(D1)}$$

which we first imagine we shall try to calculate by putting the system in a box so that the resonance associated with $\mathscr{E}_p$ becomes a set of close-lying discrete 2p-1h states in which the particle mode a is imbedded. We then model the continuum limit by replacing the δ function by a smearing function

$$\rho_\Delta(E-\mathscr{E}_p)=\frac{1}{\pi}\frac{\Delta}{\frac{1}{4}\Delta^2+(E-\mathscr{E}_p)^2}\,, \quad \text{(D2)}$$

where $\Delta\gg$ level spacing. However, it is well known from the theory of Green's functions that $|\,\Phi_p(a0)\,|^2$ is the residue at the pole $z\equiv\mathscr{E}_p$ of the one-particle Green's function $G(z)$ and the latter can be identified in a commensurate approximation as the reciprocal of the expression which annihilates $\Phi_p(a0)$, namely, the rhs of (7.23) *without the smoothing quantity* Δ. Remark that in the discrete case $G(z)$ is well defined without further assumption. This expression can be written schematically as

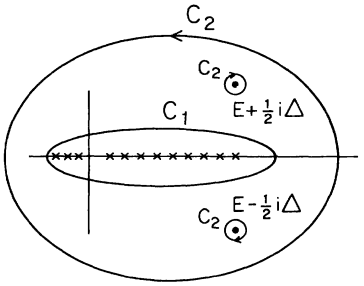

FIG. 5. Contours for the calculation of the strength function. C_1 is the original contour encircling all the poles of the Green's function. For the deformed contour C_2, nonvanishing contributions come only from the poles of the spreading function.

$$G(z)^{-1}=z-\bar{\epsilon}_a-\sum\frac{|\,V_{a\alpha}\,|^2}{z-E_\alpha}\,. \quad \text{(D3)}$$

Referring to Fig. 5, the crosses indicate the poles $\mathscr{E}_p$. The definition (D1) is therefore equivalent to the expression

$$P_a(E)=\frac{1}{\pi}\oint_{C_1}G(z)\rho(E-z)dz\,. \quad \text{(D4)}$$

Deforming the contour C_1 to infinity, we reduce the integral to the evaluation of the residues at the simple poles of the smoothing function since the contour at infinity does not contribute. We find

$$P_a(E)=\frac{1}{\pi}\mathrm{Im}\frac{1}{E+\frac{1}{2}i\Delta-\bar{\epsilon}_a-\sum\frac{|\,V_{a\alpha}\,|^2}{E+\frac{1}{2}i\Delta-E_\alpha}}$$
$$=\frac{\Gamma_a+\Delta}{(\bar{\epsilon}_a+\Delta E_a-E)^2+\frac{1}{4}(\Gamma+\Delta)^2}\,, \quad \text{(D5)}$$

where

$$\Delta E_a=\sum_\alpha\frac{|\,V_{a\alpha}\,|^2(E-E_\alpha)}{(E-E_\alpha)^2+\frac{1}{4}\Delta^2} \quad \text{(D6)}$$

and

$$\Gamma_a=\Delta\sum_\alpha\frac{|\,V_{a\alpha}\,|^2}{(E-E_\alpha)^2+\frac{1}{2}\Delta^2} \quad \text{(D7)}$$

coincide with Eqs. (7.26) and (7.27), except for notation.

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