therefore, (A3) and (A4) reduce to

$$\int dx\delta[f(x)]g(x)=[2g(x_j)/|f''(x_j)|]\int d\xi\delta(\xi^2), \quad \text{(A6)}$$

$$\int dx\delta[f(x)]g(x)\epsilon(x-x_j)=2g'(x_j)/|f''(x_j)|. \quad \text{(A7)}$$

(A7) is a finite expression, but (A6) contains the divergence,

$$\int d\xi\delta(\xi^2)=\int d\xi\delta(\xi)/|\xi|=1/|\xi| \quad \text{for} \quad \xi=0. \quad \text{(A8)}$$

To evaluate the integrals (4.5) to (4.8) it must first be noted that $\delta(z-z')^2$ is satisfied at the values of τ' for which $z=x(\tau')$ lies on a light cone of $z=x(\tau)$. Since z is a point on the world line of the charge, and the charge is assumed to move at speeds less than that of light, the only value of τ' for which the δ function is satisfied is $\tau'=\tau$. Letting

$$f(\tau')=(z-z')^2, \quad g(\tau')=\dot{z}_\mu',$$

where $f(\tau')$ has a second-order zero at $\tau'=\tau$, and applying (A6) and (A7) we obtain directly (4.5) and (4.6).

To obtain (4.7) and (4.8), we write

$$\partial eA_\nu{}^K(z)/\partial z_\mu=-e^2\int d\tau'\dot{z}_\nu'\partial[\delta(z-z')^2]/\partial z_\mu'$$

$$=-e^2\int d\tau'\frac{(z_\mu'-z_\mu)\dot{z}_\nu'}{(z_\sigma'-z_\sigma)\dot{z}_\sigma'}\frac{\partial}{d\tau'}\delta(z-z')^2$$

$$=e^2\int d\tau'\delta(z-z')^2g(\tau'), \quad \text{(A9)}$$

and similarly,

$$\partial eA_\nu{}^D(z)/\partial z_\mu=\mp e^2\int d\tau'\delta(z-z')^2\epsilon(\tau-\tau')g(\tau'), \quad \text{(A10)}$$

where

$$g(\tau')=(\partial/\partial\tau')\{(z_\mu'-z_\mu)\dot{z}_\nu'/(z_\sigma'-z_\sigma)\dot{z}_\sigma'\}. \quad \text{(A11)}$$

Expanding $g(\tau')$ in a Taylor's series about the point $\tau'=\tau$ gives

$$g(\tau')=-(\dot{z}_\mu\ddot{z}_\nu+\tfrac{1}{2}\ddot{z}_\mu\dot{z}_\nu)+(\dot{z}_\mu d\ddot{z}_\nu/dt+\ddot{z}_\mu\ddot{z}_\nu+\tfrac{1}{3}\dot{z}_\nu d\ddot{z}_\mu/dt$$
$$+\tfrac{1}{3}\dot{z}_\mu\dot{z}_\nu\dot{z}_\sigma d\ddot{z}_\sigma/dt)(\tau'-\tau)+O(\tau'-\tau)^2. \quad \text{(A12)}$$

Applying (A6) and (A7) to (A9) and (A10), we obtain directly (4.7) and (4.8).

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Generalized Hartree-Fock Approximation for the Calculation of Collective States of a Finite Many-Particle System*

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A finite many-particle system can have collective states for which the off-diagonal matrix elements of certain one-particle operators are of the same order of magnitude as the diagonal elements. In such cases it is suggested that the random-phase approximation is in need of generalization. Examples are the uniform translational motion of any system and the rotational motion of deformed nuclei. The generalization is suggested after a review and critical analysis of the Hartree-Fock approximation. The model single-particle wave functions of the latter are replaced by wave functions in a space labeled both by the particle variables and by the quantum numbers of the collective motion. These generalized amplitudes are defined field-theoretically, and a self-consistent scheme for their calculation is obtained from the equations of motion. In addition to the self-consistent potential defined in the enlarged space, the energies of the excited states also turn out to be given by a natural self-consistency requirement. The new calculational scheme is first applied to a systematic restudy of the random-phase approximation where the self-consistency requirement on the energies has previously been overlooked. As a first characteristic application we obtain without "pushing" the total mass of a system in uniform translation, and a reinterpretation of the Hartree-Fock average field.

I. INTRODUCTION AND REVIEW

OUR aim in this paper is to describe a new method for the study of certain types of collective motion characteristic of *finite* many-particle systems. The method is viewed most naturally as an extension of the Hartree-Fock approximation (HFA),[1] and we have dubbed it the generalized Hartree-Fock approximation (GHFA). Several of the most fruitful recent develop-

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[1] A recent reference from which the reader may begin to trace the literature is W. H. Adams, Phys. Rev. **127**, 1650 (1962).

ments in many-particle theory have been similarly characterized, and we shall show that our equations contain these as special cases. In particular, both the BCS theory of superconductivity[2] with its extensions to the problems of[3] liquid He^3 and of nuclear structure,[4] as well as the random-phase approximation (RPA) of Bohm and Pines[5] with its extension to include ground state correlations[6] and pairing interactions,[7] have been formulated as generalizations of the original time-independent HFA. We shall show that our equations yield all of these approximations upon specialization. But they are also capable of dealing with problems for which previous formulations are not fully adequate, such as the center-of-mass problem and the problem of nuclear rotations.

We deal concretely with a system of fermions described by annihilation and creation operators a_α and $a_\alpha^\dagger$ for an arbitrary but complete set of single-particle states α. As usual the Hamiltonian is given by[8]

$$H=(\alpha|T|\beta)a_\alpha^\dagger a_\beta+\tfrac{1}{4}(\alpha\beta|V|\gamma\delta)a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \quad (1a)$$

with

$$(\alpha|T|\beta)=(\beta|T|\alpha)^*, \quad (1b)$$

and

$$(\alpha\beta|V|\gamma\delta)=-(\beta\alpha|V|\gamma\delta)=-(\alpha\beta|V|\delta\gamma)=(\gamma\delta|V|\alpha\beta)^*. \quad (1c)$$

For orientation and a brief review, let us study the ground-state energy of the system,

$$W_N(0)=\langle 0|H|0\rangle=(\alpha|T|\beta)(\beta|\rho|\alpha)+\tfrac{1}{4}(\alpha\beta|V|\gamma\delta)\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|0\rangle, \quad (2)$$

$$(\beta|\rho|\alpha)=\langle 0|a_\alpha^\dagger a_\beta|0\rangle.$$

In the original HFA we factorize the two-particle expectation value,

$$\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|0\rangle=(\delta|\rho|\beta)(\gamma|\rho|\alpha)-(\gamma|\rho|\beta)(\delta|\rho|\alpha). \quad (3)$$

This is correct if the ground state is indeed a Slater determinant of orthonormal single-particle wave functions $\psi_i(\alpha)$, $i=1,\cdots,N$. Then

$$(\alpha|\rho|\beta)=\sum_{i=1}^{N}\psi_i(\alpha)\psi_i^*(\beta). \quad (4)$$

The HF self-consistent equations for the determination of the matrix ρ follow from the equations of motion,

$$\langle 0|[a_\beta^\dagger a_\alpha,H]|0\rangle=0, \quad (5)$$

and the factorization (3). In this formulation, the HFA appears strictly as a theory of the ground state. As is well known, however, the effective single-particle potential,

$$(\alpha|\mathcal{U}|\beta)=(\alpha\alpha'|V|\beta\beta')(\beta'|\rho|\alpha'), \quad (6)$$

serves, once it has been fixed by the N solutions $\psi_i(\alpha)$, to determine the remaining members $\psi_j(\alpha)$, $j=N+1,\cdots$, of a complete set, which can be used to construct excited states in the sense of the shell model.

The ground-state theory of a fermion superfluid follows from the extension of the assumption (3) to

$$\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|0\rangle=(\delta|\rho|\beta)(\gamma|\rho|\alpha)-(\gamma|\rho|\beta)(\delta|\rho|\alpha)+(0|\sigma^\dagger|\beta\alpha)(\delta\gamma|\sigma|0), \quad (7)$$

where the new correlation function is defined by

$$(\delta\gamma|\sigma|0)=\langle 0|a_\delta a_\gamma|0\rangle=(0|\sigma^\dagger|\delta\gamma)^*. \quad (8)$$

By the definition (8), we must understand one of two things: If we continue to work with the original Hamiltonian (1), then the two ground states indicated in $\langle 0|a_\delta a_\gamma|0\rangle$ must, of course, be distinguished in reality as those of N and $N-2$ particles in the bra and ket, respectively. On the other hand, it always turns out to be more convenient to work with $H'=H-\mu N$, where μ is the chemical potential and with the concept of a ground state in which the number of particles is not fixed. The generalized HF equations for this case, or as they have been properly called[4] the Hartree-Bogolyubov equations,[9] follow from the requirements

$$\langle 0|[a_\beta^\dagger a_\alpha,H']|0\rangle=0, \quad (9)$$

$$\langle 0|[a_\beta a_\alpha,H]|0\rangle=0, \quad (10)$$

and the assumption (7). The Hartree-Bogolyubov formulation can, by the introduction of a suitable matrix notation,[10] be cast into the same formal mold as the usual HFA. Of course, this should not obscure the profound physical difference between the cases in that an independent particle ground state has been replaced by a pair ground state of the BCS type. In the following discussion, we shall omit any further reference to the superfluid case, remembering, however, that an appropriate generalization is feasible in every instance, as we shall show in a later paper.

The next stage of development of the theory is the recognition that *even if* the ground state is reasonably represented as a simple shell-model state as determined by the average HF field, the excited states may be rather poorly approximated as regards both their energies and their wave functions. The simplest excited states are those in which we remove a particle from one

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[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[3] For example, P. W. Anderson and P. Morel, Phys. Rev. **123**, 1911 (1961).

[4] For example, M. Baranger, Phys. Rev. **122**, 992 (1962).

[5] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

[6] S. Fallieros and R. A. Ferrel, Phys. Rev. **116**, 660 (1959).

[7] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

[8] We shall almost always use the convention that repeated indices are summed. The matrix $(\alpha|T|\beta)$ represents the matrix element of the kinetic-energy operator between single-particle states $(\alpha|$ and $|\beta)$ whereas $(\alpha\beta|V|\gamma\delta)$ is the antisymmetrized matrix element of the two-body potential.

[9] N. N. Bogolyubov, Usp. Fiz. Nauk. **67**, 549 (1959) [translation: Soviet Phys.—Usp. **67**, 236 (1959)].

[10] J. G. Valatin, Phys. Rev. **122**, 1012 (1961).

of the initially occupied modes $\psi_i(\alpha)$ and place it in one of the initially unoccupied modes $\psi_j(\alpha)$. It may happen that the "residual" interaction which connects these "particle-hole" configurations induces important coherence (or collective) effects, completely absent in the averaged field approximation.

In the RPA, one considers a special class of such possibilities by studying the matrix elements $\langle 0|a_\beta^\dagger a_\alpha|n\rangle$, where in the simple shell model $|n\rangle$ can only be a particle-hole state, but where we now ask the theory to give us more accurately the class of states characterized by such nonvanishing matrix elements. The relevant equations are in this case (5) and

$$\langle 0|[a_\beta^\dagger a_\alpha, H]|n\rangle = [W_N(n) - W_N(0)]\langle 0|a_\beta^\dagger a_\gamma|n\rangle \equiv E(n)(\alpha n|\rho|\beta 0). \quad (11)$$

In evaluating the left-hand side of (11), we encounter a correlation function of the form $\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|n\rangle$. The basic approximation of the RPA is that this matrix element is well-represented by an antisymmetric factorization process

$$\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|n\rangle \cong [\langle 0|a_\beta^\dagger a_\delta|0\rangle\langle 0|a_\alpha^\dagger a_\gamma|n\rangle + \langle 0|a_\beta^\dagger a_\delta|n\rangle\langle n|a_\alpha^\dagger a_\gamma|n\rangle] - [(\delta \leftrightarrow \gamma)]. \quad (12)$$

With the additional assumption

$$\langle n|a_\alpha^\dagger a_\gamma|n\rangle \cong \langle 0|a_\alpha^\dagger a_\gamma|0\rangle, \quad (13)$$

Eq. (12) becomes

$$\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|n\rangle \cong [(\delta|\rho|\beta)(\gamma n|\rho|\alpha 0) + (\gamma|\rho|\alpha)(\delta n|\rho|\beta 0)] - [(\delta \leftrightarrow \gamma)]. \quad (14)$$

If we assume the $(\delta|\rho|\beta)$ to be given by the HFA, then with (14), (11) becomes an eigenvalue problem for the excitation energies $E(n)$ and for $(\alpha n|\rho|\beta 0)$. Before considering the rationale of (12) and (13), we also remark that they imply, simply by analogy, a generalization of (3) to

$$\langle 0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|0\rangle = [(\delta|\rho|\beta)(\gamma|\rho|\alpha) + \sum_n (\delta n|\rho|\beta 0)(\gamma 0|\rho|\alpha n)] - [(\delta \leftrightarrow \gamma)], \quad (15)$$

and the additional sums will then correspondingly modify the ground-state energy expression Eq. (2).

The *a priori* justification for (12) and (13) is based on the picture that the states $|n\rangle$ under investigation are given approximately as coherent superpositions of particle-hole configurations.[11] Whereas the nonvanishing matrix elements $(\alpha|\rho|\beta)$ are of order unity, the nonvanishing $(\alpha n|\rho|\beta 0)$ can be shown to be of order $N^{-1/2}$ for this class of coherent states. This justifies the linearization procedure (12), which supposes the off-diagonal elements to be small compared to the diagonal ones, whereas (13) follows to order N^{-1} from the fact that only one particle out of N is excited on the average.

[11] The excited particle has, however, been promoted from a ground state in which the particles are to some extent correlated.

The RPA has proved its value in the study of the excited states of an infinite medium[5–7] as well as in the study of certain classes of excited states in finite systems, notably for various kinds of vibrational states of nuclei.[12]

The major new feature of this paper is a treatment of important types of collective excitations for which the linearization process (12) and (13) is inadequate. We illustrate by an example which served as the starting point of the work, i.e., the rotational spectrum of deformed nuclei. Let $|n\rangle$ here represent any member of the rotation band of the ground state of an even-even nucleus, so that $|0\rangle$ is a *spherically symmetric* state. Let the a_α be destruction operators for particles of definite angular momentum. It follows that only the elements $(\alpha|\rho|\beta)$ with $\alpha=\beta$ are nonvanishing, and this means that the HFA as formulated in Eqs. (3)–(5) cannot possibly yield a deformed-well shell model, known to be a sound basis for the understanding of many nuclear properties in the region of deformed nuclei.[13]

A formal way out of this dilemma is not difficult to find. We simply put on blinders and replace $|0\rangle$ by $|0, \text{deformed}\rangle$, i.e., we lift the restriction that the ground state be one of definite angular momentum. The theory that then emerges from (3)–(5) can have solutions corresponding to the deformed-well model. But now we must certainly probe more deeply the significance of the increased freedom we have allowed ourselves in the choice of trial function. Its meaning is, in fact, well known.[14] Since the energy differences between neighboring states of the band $|n\rangle$ are quite small compared to the total binding energy of the ground state, it appears reasonable to allow as a trial function the form

$$|0, \text{deformed}\rangle = \sum_I A(I)|I\rangle, \quad (16)$$

i.e., a superposition of states with different rotation symmetry.

In so far as we now find a solution $(\alpha|\rho|\beta)$ with important elements $\alpha \neq \beta$, this has the clear implication that we are dealing with a physical problem for which there are matrix elements $\langle n|a_\beta^\dagger a_\alpha|n'\rangle$, $n \neq n'$, of the same order of magnitude as the diagonal elements and, in particular, as $\langle 0|a_\beta^\dagger a_\alpha|0\rangle$.

In this paper we begin the development of a theory which incorporates such a possibility from the outset and thus goes beyond both the HFA and the RPA. We shall attempt to establish that the basic equations may be cast in the form

$$\langle n'|[a_\beta^\dagger a_\alpha, H]|n\rangle \equiv [E(n) - E(n')](\alpha n|\rho|\beta n'), \quad (17)$$

[12] For example, G. Brown, A. Evans, and D. J. Thouless, Nucl. Phys. **24**, 1 (1961).

[13] For a recent summary, see B. R. Mottelson and S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Skrifter No. 8 (1959).

[14] R. E. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957); see also A. K. Kerman, *Nuclear Reactions* (Interscience Publishers, Inc., New York, 1959), Vol. I.

together with the generalized factorization

$$\langle n'|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma|n\rangle=\sum_{n''}\{(\delta n''|\rho|\beta n')(\gamma n|\rho|\alpha n'')-(\gamma n''|\rho|\beta n')(\delta n|\rho|\alpha n'')\}. \quad (18)$$

We emphasize once again that all previous approximations can be extracted from (17) and (18). In order to illustrate the extended range of application of these equations, we have in this first paper applied (17) and (18) to the problem of uniform-translational motion and shown how to compute the total mass of a system without "pushing." A natural interpretation of the average potential is also obtained. Similarly, we shall show in a subsequent paper how to extract nuclear moments of inertia without "cranking." The possibility of carrying out this program follows from the fact that Eq. (17) contains precisely those energy differences between rotational states which are suppressed in the deformed-well model. We shall see, however, that in contrast to the RPA, Eq. (17) does not yield an eigenvalue problem, but rather the $E(n)$ must be computed directly from the expression

$$W_N(0)+E(n)=\langle n|H|n\rangle, \quad (19)$$

evaluated in an approximation based on (18). This is formulated as a self-consistency requirement among (17), (18), and (19). This self-consistency requirement, as we shall show, also plays a role in the RPA, where it has previously been overlooked.

We begin our study in Sec. II with a review of the HFA. At the end of the section a derivation of the HFA is presented, which, though superficially clumsy as a form of argumentation, has the virtue of suggesting the direction to be taken for generalization. Section III then contains the complete statement of the formal generalization we propose, the GHFA. In Sec. IV, we derive the RPA as a special class of solutions of the GHFA. Here we have found at least one novel result in that the self-consistency condition mentioned above is seen to imply a different normalization condition for the RPA amplitudes. Finally, Sec. V contains a study of the problem of translation. The equation of the GHFA are solved exactly for this case and shown to yield the correct total mass of the system. The same result is then achieved by an approximation method which will serve as a prototype for future applications.

Appendix A reviews the question of local stability[15] of a solution of the HFA. In Appendix B, we discuss a preliminary variational formulation of the GHFA. Finally, Appendix C is devoted to a study of the zero-energy solutions of the RPA.

II. THE HARTREE-FOCK METHOD

We devote this section to a review of largely well-known results in the theory of the self-consistent field approximation. This will provide us with a corpus of classical results with which to compare the extensions to be proposed later. It will also serve to introduce those methods of reasoning which suggest most naturally the generalizations in question. We begin with the operator equations of motion which follow from the Hamiltonian (1),

$$[a_\alpha,H]=(\alpha|T|\beta)a_\beta+\tfrac{1}{2}(\alpha\beta|V|\gamma\delta)a_\beta^\dagger a_\delta a_\gamma, \quad (20)$$

$$[a_\alpha^\dagger,H]=-(\alpha|T|\beta)^*a_\beta^\dagger-\tfrac{1}{2}(\alpha\beta|V|\gamma\delta)^*a_\gamma^\dagger a_\delta^\dagger a_\beta. \quad (21)$$

As an example of[16] Eq. (20) we study the matrix elements $\langle i|a_\alpha|0\rangle$ connecting the ground state $|0\rangle$ of the system of N particles with one of the eigenstates $|i\rangle$ of the $N-1$ particle system. Let $W_N(0)$ and $W_{N-1}(i)$ be the associated energy values with

$$\mathcal{E}_i=W_N(0)-W_{N-1}(i). \quad (22)$$

From (20) we then obtain (no sum on i understood)

$$[\mathcal{E}_i\delta_{\alpha\beta}-(\alpha|T|\beta)]\langle i|a_\beta|0\rangle=\tfrac{1}{2}(\alpha\beta|V|\gamma\delta)\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle. \quad (23)$$

To arrive at the self-consistent field approximation, we set

$$(\alpha\beta|V|\gamma\delta)\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle\cong 2(\alpha\beta|V|\gamma\delta)\times\langle 0|a_\beta^\dagger a_\delta|0\rangle\langle i|a_\gamma|0\rangle, \quad (24)$$

which is equivalent to the factorization (3). We return below to further discussion of this step, proceeding for the moment in as straight a line as possible. In terms of the single-particle density matrix $(\alpha|\rho|\beta)$ of Eq. (2), and the Hartree-Fock self-consistent field $(\alpha|\mathcal{U}|\beta)$ of Eq. (6), Eq. (23) becomes

$$[\mathcal{E}_i\delta_{\alpha\beta}-(\alpha|T|\beta)]\langle i|a_\beta|0\rangle=(\alpha|\mathcal{U}|\beta)\langle i|a_\beta|0\rangle, \quad (25)$$

or with

$$(\alpha|\mathcal{H}|\beta)\equiv(\alpha|(T+\mathcal{U})|\beta), \quad \psi_i(\alpha)\equiv\langle i|a_\alpha|0\rangle, \quad (26)$$

$$\mathcal{E}_i\psi_i(\alpha)=(\alpha|\mathcal{H}|\beta)\psi_i(\beta). \quad (27)$$

Equation (27) represents an equivalent single-particle problem, rendered closed, but nonlinear, through the circumstances that $\mathcal{H}$ is itself a functional of the vectors $\psi_i(\alpha)$, since

$$(\alpha|\rho|\beta)=\sum_i\langle 0|a_\beta^\dagger|i\rangle\langle i|a_\alpha|0\rangle=\sum_i\psi_i(\alpha)\psi_i^*(\beta). \quad (28)$$

The problem is, however, still not sufficiently well defined by (27) and the associated definitions. Since for a given $\mathcal{H}$, (27) generates an infinite set of mutually orthogonal solutions ψ_a[17]

$$\sum_\alpha\psi_a^*(\alpha)\psi_{a'}(\alpha)=0, \quad a\neq a', \quad (29)$$

[15] D. J. Thouless, Nucl. Phys. **21**, 225 (1960).

[16] Though in the Introduction we have emphasized the density matrix, the reader will observe that in the body of the paper, we emphasize the computation of HF wave functions.

[17] The index a will refer to a complete set of modes, whereas the indices i and j will refer to modes occupied and unoccupied, respectively, in the N-particle ground state.

which set may be used in turn to yield via (28) the next approximation to $\mathcal{H}$, it is clear that the ultimate solution will depend on the number of $\psi_i(\alpha)$ used in (28), as well as on the norm assigned each one. The conditions which provide this information are

$$\sum_\alpha \langle 0|a_\alpha^\dagger a_\alpha|0\rangle = \sum_\alpha (\alpha|\rho|\alpha) = \mathrm{tr}\rho = N, \quad (30)$$

and the assertion that ρ is a projection operator,

$$\rho^2 = \rho. \quad (31)$$

Equation (30) expresses the conservation of particles, whereas (31) may be established by studying the matrix element of the anticommutation relations,

$$\delta_{\alpha\beta} = \langle 0|\{a_\beta^\dagger, a_\alpha\}|0\rangle = \sum_i \psi_i(\alpha)\psi_i^*(\beta) + \sum_j \phi_j(\alpha)\phi_j^*(\beta),$$
$$\phi_j(\alpha) = \langle 0|a_\alpha|j\rangle. \quad (32)$$

The wave functions $\phi_j(\alpha)$, the particle modes, satisfy (to order N^{-1}) the same equation as the $\psi_i(\alpha)$, as can be shown by repeating the reasoning given for the latter and, therefore, are included in the orthogonality relation (29) since the associated eigenvalues are distinct from those of the $\psi_i(\alpha)$. From (32) and the definition

$$(\alpha|\tau|\beta) = \sum_j \phi_j(\alpha)\phi_j^*(\beta), \quad (33)$$

now follows (31) and, in addition, the equation

$$\tau^2 = \tau, \quad (34)$$

since $\rho\tau = 0$.

Equation (31) yields the result that the $\psi_i(\alpha)$ are normalized and (30) then provides the supplementary information that we must construct ρ from precisely N such solutions. We have thus *derived* that $|0\rangle$ and $|i\rangle$ are the Slater determinants

$$|0\rangle = \prod_{i'=1}^{N} b_{i'}^\dagger \Phi_0, \quad |i\rangle = \prod_{i' \neq i} b_{i'}^\dagger \Phi_0,$$
$$b_i^\dagger = a_\alpha^\dagger \psi_i(\alpha), \quad (35)$$

and Φ_0 is the vaccum state. From (35) we see that the $b_i^\dagger$ are the creation operators for the eigenvectors ψ_i of $\mathcal{H}$. In general to obtain the ground state we choose the N lowest eigenvalues of (27).[18] The associated $\psi_i(\alpha)$ then determine a $\mathcal{U}$ from which the remaining members $\psi_j(\alpha) = \phi_j(\alpha)$, $j = N+1, \cdots$, of the complete set may be determined.

We can compute the energy of the ground state in the same approximation by using Eqs. (1) and (3),

$$W_N(0) = \langle 0|H|0\rangle = (\alpha|T|\beta)(\beta|\rho|\alpha) + \tfrac{1}{2}(\alpha\beta|V|\gamma\delta)(\delta|\rho|\beta)(\gamma|\rho|\alpha)$$
$$= \mathrm{tr}[T\rho + \tfrac{1}{2}\mathcal{U}\rho]$$
$$= \mathrm{tr}[T\sum_i \psi_i\psi_i^\dagger + \tfrac{1}{2}V(\sum_i \psi_i\psi_i^\dagger) \times (\sum_{i'} \psi_{i'}\psi_{i'}^\dagger)]. \quad (36)$$

The last form of (36) is a convenient basis for a second (and best known) characterization of the HF equations as those which determine a stationary point of (36) upon the variation of the $\psi_i^\dagger$, ψ_i subject to a conserved norm[19] $\|\psi_i\|^2 = (\psi_i, \psi_i) = 1$. Yet a third equivalent characterization, that described in Sec. I, is the statement that

$$[\rho, \mathcal{H}] = 0, \quad (37)$$

subject to (30) and (31). Here (37) replaces (27) from which it may be readily deduced. Thus, the HFA is also characterized by the requirement that ρ and $\mathcal{H}$ be simultaneously brought to diagonal form, the "first N" eigenvalues of $\mathcal{H}$ corresponding to the eigenvalue unity of ρ, the remaining ones to the eigenvalue zero. In Appendix A we have included a review of the stability theory of the HFA.

To conclude this section, we return to a critical study of the derivation of the HF theory. To this point, we have availed ourselves only of the standard derivations, as expressed, for example, in the factorizations (3) or (24) which commit us irrevocably to a Slater determinantal wave function. We present here another mode of reasoning for which we at least claim the virtue that it *suggested* the generalization to be developed in the next section. In order to be able to use a general form of argument, we assume that a summation over a single-particle label α is of order N. For $(\alpha\beta|V|\gamma\delta)$ we must suppose either that it is proportional to N^{-2} or, equivalently (the more usual case in practice), to N^{-1} but that there is a conservation law which fixes the fourth index, given the other three.

From these considerations alone, one may draw qualitative conclusions concerning the order of magnitude of the matrix elements in our basic Eq. (23), using only the requirement that both sides be the same order of magnitude:

(1) In most cases, i.e., for the order of N values of each of the indices, $\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle \sim N^{-1}\langle i|a_\beta|0\rangle$. This is, for example, the order of magnitude given by perturbation theory based upon an unperturbed single-particle picture. Equivalently, this means that omitting a single term from the summation has no effect on the properties of the system for N large. Assuming for definiteness the case $V \sim N^{-1}$, the total number of such terms is $O(N^2)$.

(2) We must, more generally, allow the possibility that for some values of the indices $\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle \sim N^{-\mathcal{K}}\langle i|a_\beta|0\rangle$, where for fermions $\mathcal{K} \geq 0$. In this case the total number of terms on the right-hand side of (23) is $0(N^{1+\mathcal{K}})$. The realization of the case $\mathcal{K} = 0$ corresponds precisely to the possibility of defining an HFA of some kind. The possible occurrence of values of $\mathcal{K}$ intermediate between 0 and 1 will not be considered here. For our present purposes we separate $\mathcal{K} = 0$ from all other possible choices.

[18] Possible exceptions to this remark are discussed in Ref. 1.

[19] We need not insist on the mutual orthogonality of the Ψ_i since this emerges from the equations.

We now study a particular class of terms of the $\mathcal{K}=0$ type, namely those which yield the HFA. Consider the right-hand side of (23). For a given β, we suppose that the case $\mathcal{K}=0$ obtains if either δ or γ takes a subset β' of values, necessarily small in number compared to N. To an error of the order of N^{-1} we may therefore write,

$$\sum_{\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle$$
$$=2\sum_{\beta\gamma\beta'}(\alpha\beta|V|\gamma\beta')\langle i|a_\beta^\dagger a_{\beta'}a_\gamma|0\rangle + \sum_{(\gamma,\delta)\neq\beta'}(\alpha\beta|V|\gamma\delta)\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle. \quad (38)$$

The HFA emerges from the additional assumptions that[20] $\langle i|a_\beta^\dagger a_{\beta'}a_\gamma|0\rangle\cong\langle i|a_\gamma a_\beta^\dagger a_{\beta'}|0\rangle$ is large only because the diagonal matrix element $\langle 0|a_\beta^\dagger a_{\beta'}|0\rangle$ is large $\sim O(1)$, so that we may write

$$\langle i|a_\gamma a_\beta^\dagger a_{\beta'}|0\rangle\equiv\sum_n\langle i|a_\gamma|n\rangle\langle n|a_\beta^\dagger a_{\beta'}|0\rangle \cong\langle i|a_\gamma|0\rangle\langle 0|a_\beta^\dagger a_{\beta'}|0\rangle, \quad (39)$$

and, finally, that the second term of (38) may be neglected compared to the first. Since on general grounds, the two terms of (38) are of the same order of magnitude, this latter neglect requires further detailed study, which goes beyond the scope of this work.[21] Qualitatively though, one may recognize the possibility that in favorable cases the many contributions to the second term of (38) will add incoherently and, therefore, tend largely to cancel one another.

With the above assumptions, we have reached the representation

$$\sum_{\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle\cong 2\sum_{\beta\gamma\beta'}(\alpha\beta|V|\gamma\beta')\times\langle 0|a_\beta^\dagger a_{\beta'}|0\rangle\langle i|a_\gamma|0\rangle. \quad (40)$$

This becomes equivalent to (24), upon which our derivation was originally based, as soon as we realize that we may now sum freely over $\beta'=\delta$, since the terms thereby added must by our previous reasoning be small. Having now rederived the usual HFA, we show in the next section how the reasoning just given may be generalized.

III. THE GENERALIZED HARTREE-FOCK APPROXIMATION

The generalization to be studied[22] will be based on the decomposition (38) or analogous formulas in which only the first term on the right-hand side is retained. This means that the resulting theory will not apply to systems with superfluid behavior. The required extension is, however, relatively straightforward and will be developed in a later paper. We, therefore, assume that

$$\sum_{\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)\langle i|a_\beta^\dagger a_\delta a_\gamma|0\rangle=2\sum_{\beta\gamma\beta'}(\alpha\beta|V|\gamma\beta')\times\langle i|a_\gamma a_\beta^\dagger a_{\beta'}|0\rangle. \quad (41)$$

In contrast to the approximation (39), we shall now suppose that there exist (a small number of) excited states $|n\rangle$ for which

$$\langle n|a_\beta^\dagger a_{\beta'}|0\rangle\sim\langle 0|a_\beta^\dagger a_{\beta'}|0\rangle. \quad (42)$$

Physically, this means that there are one-particle operators with off-diagonal matrix elements as important as their diagonal elements, and these enter importantly in the energy. Thus, we have to allow that

$$\langle i|a_\gamma a_\beta^\dagger a_{\beta'}|0\rangle=\sum_n\langle i|a_\gamma|n\rangle\langle n|a_\beta^\dagger a_{\beta'}|0\rangle \equiv\sum_n\psi_i(\gamma n)(\beta'0|\rho|\beta n). \quad (43)$$

In place of the HF Eq. (25), we now obtain the equation

$$[\mathcal{E}_i\delta_{\alpha\beta}-(\alpha|T|\beta)]\psi_i(\beta 0)=(\alpha 0|\mathcal{U}|\beta n)\psi_i(\beta n), \quad (44)$$

where

$$(\alpha 0|\mathcal{U}|\beta n)=(\alpha\gamma|V|\beta\delta)(\delta 0|\rho|\gamma n). \quad (45)$$

We are, thus, confronted with the obvious fact that the system of Eqs. (44) is incomplete. To obtain a closed system, we must study the equation of motion (20) for the matrix element $\psi_i(\alpha n)=\langle i|a_\alpha|v\rangle$. Toward this end, we define

$$W_N(n)-W_{N-1}(i)=[W_N(n)-W_N(0)]+[W_N(0)-W_{N-1}(i)] \equiv E(n)+\mathcal{E}_i \quad (46)$$

and generalize the factorization (43) by writing

$$\langle i|a_\gamma a_\beta^\dagger a_{\beta'}|n\rangle=\sum_{n'}\langle i|a_\gamma|n'\rangle\langle n'|a_\beta^\dagger a_{\beta'}|n\rangle \equiv\sum_{n'}\psi_i(\gamma n')(\beta' n|\rho|\beta n'), \quad (47)$$

basing it on assumptions analogous to (42). Starting from (20) we then find the closed system of equations

$$[\mathcal{E}_i\delta_{nn'}\delta_{\alpha\beta}+E(n)\delta_{nn'}\delta_{\alpha\beta}-(\alpha|T|\beta)\delta_{nn'}]\psi_i(\beta n') =(\alpha n|\mathcal{U}|\beta n')\psi_i(\beta n'), \quad (48)$$

with a GHF potential

$$(\alpha n|\mathcal{U}|\beta n')=(\alpha\gamma|V|\beta\delta)(\delta n|\rho|\gamma n'). \quad (49)$$

The precise sense in which (48) and (49) constitute a closed system of equations and the kind of solutions to be sought thereto requires further specification. We first note that (48) can be rendered in a condensed form, comparable to (37),

$$\mathcal{E}_i\psi_i(\alpha n)=(\alpha n|\mathcal{K}|\beta n')\psi_i(\beta n'), \quad (50)$$

[20] The commutation involved in this step is equivalent to the assumption that the HF potential for a system of $N-1$ particles is sensibly the same as that for N particles. Thus, the error is of relative order N^{-1}.

[21] The definition of the first term of (38) is sufficiently general as to include both the RPA and GHFA. A systematic theory of higher order effects, such as contained in the second term of (38) is in the course of development. See H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961); C. Fano and J. Sawicki, Nuovo Cimento **20**, 586 (1962). For an alternative method, see G. Do Dang and A. Klein, Phys. Rev. **130**, 2572 (1963).

[22] A preliminary report has been given by A. K. Kerman and A. Klein, Phys. Letters **1**, 185 (1962).

where the GHF Hamiltonian, defined in an enlarged space designated both by the single-particle labels α and by the quantum numbers n of the excited states, is here given by

$$(\alpha n|\mathcal{H}|\beta n')=-E(n)\delta_{nn'}\delta_{\alpha\beta}+(\alpha|T|\beta)\delta_{nn'}+(\alpha n|\mathcal{U}|\beta n'). \quad (51)$$

The GHF potential $\mathcal{U}$ is known from (49) if the solutions to (50) are known, since

$$(\delta n|\rho|\gamma n')=\langle n'|a_\gamma^\dagger a_\delta|n\rangle=\sum_i \psi_i(\delta n)\psi_i^*(\gamma n'). \quad (52)$$

This aspect of the self consistency generalizes immediately that encountered in the traditional HFA. According to (51), we must, however, also specify the $E(n)$ in order to solve (50). Of the solution to the latter equation, we must then require that it reproduce the $E(n)$ fed in initially. We must therefore seek additional self-consistency requirements. The form taken by these is to be given below [Eq. (60)]. We may already assert, however, that our method, if proven viable, will constitute *a GHFA for the computation of the energies of classes of excited states of a many-body system.*

Before completing the justification for this assertion, let us backtrack a moment and seek conditions on the solutions $\psi_i(\alpha n)$, analogous to those contained in (29), (30), and (31). Since $\mathcal{H}$ is Hermitian, we certainly have

$$\sum_{\alpha,n}\psi_i^*(\alpha n)\psi_{i'}(\alpha n)=0, \quad i\neq i'. \quad (53)$$

In analogy with (30) we also have

$$\sum_\alpha(\alpha n|\rho|\alpha n')=\langle n|\sum_\alpha a_\alpha^\dagger a_\alpha|n'\rangle=N\delta_{nn'}. \quad (54)$$

The direct generalization of (31), the statement that ρ is a projection operator, fails to hold, however, in the present theory. This is best seen by attempting to duplicate the steps in its derivation. Instead of (32) we have

$$\langle n|\{a_\beta^\dagger,a_\alpha\}|n'\rangle=\sum_i\psi_i(\alpha n)\psi_i^*(\beta n')+\sum_j\phi_j(\alpha n')\phi_j^*(\beta n)=\delta_{\alpha\beta}\delta_{nn'}, \quad (55)$$

where

$$\phi_j(\alpha n')=\langle n'|a_\alpha|j\rangle, \quad (56)$$

will again represent the modes associated with an added particle. Two properties of (55) and (56), absent in the simple HF case, complicate the present situation. First we note that the collective quantum numbers n and n' interchange roles in the two terms of (55). More fundamental is the observation that the modes $\psi_i(\alpha n)$ and $\phi_j(\alpha n)$ no longer satisfy the same equations and, therefore, fail to be orthogonal. In contrast to (50) and (51), a comparable derivation yields the equations

$$\mathcal{E}_j\phi_j(\alpha n)=(\alpha n|\mathcal{K}|\beta n')\phi_j(\beta n'), \quad (57)$$

where

$$(\alpha n|\mathcal{K}|\beta n')=E(n)\delta_{nn'}\delta_{\alpha\beta}+(\alpha|T|\beta)\delta_{nn'}+(\alpha n'|\mathcal{U}|\beta n), \quad (58)$$

and

$$\mathcal{E}_j-E(n)=W_{N+1}(j)-W_N(n). \quad (59)$$

We must therefore be content with (55) instead of the more perspicuous Eq. (31).

Nevertheless, study of particular cases will show that (54) and (55) together provide the information previously supplied by (30) and (31). It should be clear, however, that we will be forced to study the hole modes $\psi_i(\alpha n)$ in conjunction with the particle modes $\phi_j(\alpha n)$ since they are now inextricably coupled by the normalization condition (55).

To complete the theoretical framework then, it remains only to specify the self-consistency conditions on the energy differences. But these are given naturally by the condition[23]

$$W_N(0)+E(n)=\langle n|H|n\rangle=(\alpha|T|\beta)(\beta n|\rho|\alpha n)+\tfrac{1}{2}\sum_{n'}(\alpha\beta|V|\gamma\delta)\times(\delta n|\rho|\beta n')(\gamma n'|\rho|\alpha n), \quad (60)$$

where the factorization (18), equivalent to (47), has been employed. To summarize, we must solve (50) and (57), subject to the self-consistency conditions (49) and (60) with the restrictions (54) and (55) on the nature of the solutions.

Once we have obtained the solution we will have determined the collective energies $E(n)$ and also the density matrix $(\alpha n|\rho|\alpha' n')$ which will enable us to compute all the single-particle matrix elements between the collective states (n). And finally the "wave functions" $\psi_i(\alpha n)$ give us the partial parentage between the collective states (n) of the N-particle system and the coupled collective and hole states (i) of the $(N-1)$ particle system.

In Appendix B we present a possible variational approach to the GHFA.

IV. THE RANDOM-PHASE APPROXIMATION

We devote the remainder of this paper to applications of the GHFA. In the present section which is largely though not completely a review, we show how to regain the RPA, heretofore the only systematic method available for the study of excited states. Toward this end we write our fundamental GHF equation in the explicit form

$$[\mathcal{E}_{im}+E(n)]\psi_{im}(\alpha n)=(\alpha|T|\alpha')\psi_{im}(\alpha' n)+(\alpha\beta|V|\alpha'\beta')\times[\sum_{i'm'}\psi_{i'm'}(\beta' n)\psi_{i'm'}^*(\beta n')]\psi_{im}(\alpha' n'), \quad (61)$$

where the former index (i) has been written as a double

[23] To be complete we should also study the off-diagonal quantities $\langle n|H|n'\rangle$ using the factorization (18), which should of course be zero for $n\neq n'$. These conditions are generally satisfied identically when the states n and n' differ in symmetry (for example, linear or angular momentum).

index (im) to take account of the new degree of freedom (n) in the wave functions.

In the RPA the ground state is taken to be essentially of the HF type, with, however, small amplitudes for finding configurations with single particle-hole pairs, i.e., configurations in which one particle has been promoted from below to above the Fermi surface. In the usual RPA, amplitudes for double excitation are neglected. The expectation value of a typical one-particle operator in the ground state is then $O(N)$. The excited states of interest are those formed by a coherent superposition (of the order of N terms) of particle-hole configurations. From normalization considerations a typical coefficient for a particle-hole amplitude is $O(N^{-1/2})$. It follows that a typical one-particle operator has matrix elements which are $O(N^{1/2})$. This coherence (see below) is brought about by the residual interaction not contained in the original HFA, since in the latter the corresponding excited states are single particle-hole configurations. For this simple type of state the one-particle matrix elements are $O(1)$.

It is, furthermore, assumed for large N that the neighboring systems of $N+1$ and $N-1$ particles have corresponding coherent excited states differing only by the addition or removal of a particle in one of the HF modes. Thus, we write

$$\mathcal{E}_{im}\cong\mathcal{E}_i-E(m)\,, \tag{62}$$

where it is implied that the $\mathcal{E}_i$ are approximately the unperturbed HF energies and the $E(m)$ are the same set as the $E(n)$, all this to an accuracy of relative order N^{-1}.

With this picture we write

$$\psi_{i0}(\alpha 0)\cong\psi_{in}(\alpha n)\equiv\psi_i(\alpha)\,, \tag{63}$$

$$\psi_{i0}(\alpha n)=\phi_j(\alpha)\xi_{ji}(n)\,, \tag{64}$$

$$\psi_{in}(\alpha 0)=\phi_j(\alpha)\eta_{ji}(n)\,. \tag{65}$$

As before, the i refer to occupied, the j to unoccupied modes. The proof that the ξ and η amplitudes can be so restricted is given below. From the previous qualitative discussion, the ξ_{ji} and η_{ji} are $O(N^{-1/2})$. The η_{ji} are nonvanishing only in virtue of the fact that the ground state is not pure HF and describe therefore the ground-state correlations.

By systematic exploitation of the assumptions stated above, it is a straightforward matter to deduce from (61) the equations satisfied by the amplitudes defined in Eqs. (63)–(65). For the latter two amplitudes, we obtain in first order the equations

$$\begin{aligned}&[\mathcal{E}_i-\mathcal{E}_j+E(n)]\xi_{ji}(n)\\&\quad=\phi_j^*(\alpha)(\alpha n|\mathcal{V}|\beta 0)\psi_i(\beta)\\&\quad=(ji'|V|ij')\xi_{j'i'}(n)+(jj'|V|ii')\eta_{j'i'}^*(n)\,,\end{aligned} \tag{66}$$

$$\begin{aligned}&[\mathcal{E}_i-\mathcal{E}_j-E(n)]\eta_{ji}^*(n)\\&\quad=\psi_i^*(\alpha)(\alpha n|\mathcal{V}|\beta 0)\phi_j(\beta)\\&\quad=(ij'|V|ji')\eta_{j'i'}^*(n)+(ii'|V|jj')\xi_{j'i'}(n)\,.\end{aligned} \tag{67}$$

The equation for the amplitude $\psi_i(\alpha)$, on the other hand, shows that the latter deviates from the simple HF wave function by terms of the second order in the small amplitudes ξ, η. Only this qualitative result is needed in the sequel.

Equations (66) and (67) are the standard form of the RPA.[12] We must recognize, however, that the usual justification for choosing only particle-hole configurations ξ_{ji}, η_{ji}, and setting $\xi_{i'i}$, $\eta_{i'i}=0$ is based on the extended use of Eq. (31). The latter has been replaced by the more generally applicable condition (55) which forces us to consider hole and particle excitation on a relatively equal footing. To test the equivalence of the present theory to the conventional one we must study the particle modes, i.e., the equations for the $\phi_{jm}(\alpha n)$, examine the consequences of the supplementary conditions (54) and (55), and understand the role of the self-consistency condition (60), especially in light of the fact that Eqs. (66) and (67) define an eigenvalue problem for the $E(n)$. Only after having satisfied ourselves on all these points shall we return to the eigenvalue problem, the usual focus of interest.

To launch this program we first write, in analogy with Eqs. (64) and (65)

$$\phi_{j0}(\alpha n)=\psi_i(\alpha)\mu_{ij}(n)\,, \tag{68}$$

$$\phi_{jn}(\alpha 0)=\psi_i(\alpha)\nu_{ij}(n)\,. \tag{69}$$

From (57) and (58) we then find to first order

$$(\mathcal{E}_j-\mathcal{E}_i-E(n))\mu_{ij}(n)=\psi_i(\alpha)(\alpha 0|\mathcal{V}|\beta n)\phi_j(\beta)\,, \tag{70}$$

$$(\mathcal{E}_j-\mathcal{E}_i+E(n))\nu_{ij}^*(n)=\phi_j^*(\alpha)(\alpha 0|\mathcal{V}|\beta n)\psi_i(\beta)\,. \tag{71}$$

Comparison of (70) with (66) and (71) with (67) shows that

$$\xi_{ji}(n)=-\mu_{ij}^*(n)\,, \tag{72}$$

$$\eta_{ji}^*(n)=-\nu_{ij}(n)\,. \tag{73}$$

This identification will play an essential role in the study of the supplementary conditions (54) and (55) to which we now turn.

With the help of these conditions we shall first justify the restrictions placed on the summations in (64), (65), (68), and (69). We, therefore, provisionally extend the summations in these equations over both particle and hole modes. With the help of (72) and (73), we find for an off-diagonal element of (55)

$$\begin{aligned}0&=\langle 0|\{a_\beta^\dagger,a_\alpha\}|n\rangle\\&=\psi_{i'}(\alpha)\psi_i^*(\beta)[\xi_{i'i}(n)+\eta_{ii'}^*(n)]\\&\qquad+\phi_{j'}(\alpha)\phi_j^*(\beta)[\xi_{jj'}(n)+\eta_{j'j}^*(n)]\,,\end{aligned} \tag{74}$$

or

$$\xi_{i'i}(n)+\eta_{ii'}^*(n)=\xi_{jj'}(n)+\eta_{j'j}^*(n)=0\,. \tag{75}$$

Though these conditions are sufficient to ensure that Eqs. (66) and (67), for example, would be unmodified by the extended summations, there would still remain the additional equations for the individual amplitudes in (75). That the latter vanish separately in the present

approximation follows from conditions of the type ($i \neq i'$)

$$\langle i|b_{i'}b_{i'}^{\dagger}|i\rangle=\sum_n \langle i|b_{i'}|n\rangle\langle n|b_{i'}^{\dagger}|i\rangle = \sum_n |\xi_{i'i}(n)|^2=0. \tag{76}$$

Here we have used the HF value of the initial matrix element and the definition

$$\langle i|b_{i'}|n\rangle=\xi_{i'i}(n), \tag{77}$$

which follows from (64) (summation extended to include both particles and holes) and the definition (35) of the eigenmode operators b_i. A similar argument yields $\xi_{jj'}=0$.

The diagonal elements of (55), on the other hand, contain important information concerning the renormalization of amplitudes to second order. If we write

$$\langle i|a_\alpha|0\rangle=\psi_i(\alpha)=A_i\psi_i^{(0)}(\alpha)+\delta\psi_i(\alpha), \tag{78}$$

where $\psi_i^{(0)}(\alpha)$ is the normalized HF solution, $\delta\psi_i$ is both second order in the ξ, η and orthogonal to $\psi_i^{(0)}(\alpha)$, and correspondingly for $\delta\phi_j(\alpha)$ in

$$\phi_j(\alpha)=A_j\phi_j^{(0)}(\alpha)+\delta\phi_j(\alpha). \tag{79}$$

We can thus calculate

$$\begin{aligned}\langle 0|\{a_\beta^{\dagger},a_\alpha\}|0\rangle=\delta_{\alpha\beta}=&\sum_i |A_i|^2\psi_i^{(0)}(\alpha)\psi_i^{(0)*}(\beta)\\ &+\sum_i [\delta\psi_i(\alpha)\psi_i^{(0)*}(\beta)+\psi_i^{(0)}(\alpha)\delta\psi_i^*(\beta)]\\ &+\sum_{iji'n}\phi_j(\alpha)\phi_{j'}^*(\beta)\eta_{ji}(n)\eta_{j'i}^*(n)\\ &+\sum_j |A_j|^2\phi_j^{(0)}(\alpha)\phi_j^{(0)*}(\beta)\\ &+\sum_j [\delta\phi_j(\alpha)\phi_j^{(0)*}(\beta)+\phi_j^{(0)}(\alpha)\delta\phi_j^*(\beta)]\\ &+\sum_{ii'jn}\psi_i^{(0)}(\alpha)\psi_{i'}^{(0)*}(\beta)\eta_{ji}^*(n)\eta_{ji'}(n).\end{aligned} \tag{80}$$

In obtaining (80) use has been made of (65), (69), and (73). From (80), we can conclude the important result

$$|A_i|^2=1-\sum_{jn}|\eta_{ji}(n)|^2. \tag{81}$$

Notice that (81) is equivalent to the statement

$$\begin{aligned}1&=\sum_\alpha \psi_i^*(\alpha)\psi_i(\alpha)+\sum_{\alpha n}\psi_{in}^*(\alpha 0)\psi_{in}(\alpha n)\\ &=\sum_\alpha \langle 0|a_\alpha^{\dagger}|i\rangle\langle i|a_\alpha|0\rangle\\ &\quad+\sum_{\alpha n}\langle 0|a_\alpha^{\dagger}|in\rangle\langle in|a_\alpha|0\rangle.\end{aligned} \tag{82}$$

If we sum over i and suppose the latter, as in the simple HFA, taken on N possible values, we find, using completeness,

$$N=\sum_\alpha \langle 0|a_\alpha^{\dagger}a_\alpha|0\rangle. \tag{83}$$

With the normalization (81) we have thus conserved particles in the ground state.

It is also necessary to study the corresponding normalization condition for an excited state n. We now write

$$\psi_{in}(\alpha n)=A_i(n)\psi_i^{(0)}(\alpha)+\delta\psi_{in}(\alpha n), \tag{84}$$

allowing a possible dependence of the normalization on the state n and still requiring consistently that $\delta\psi_{in}(\alpha n)$ be of second order and orthogonal to $\psi_i^{(0)}(\alpha)$. By studying the equation

$$\delta_{\alpha\beta}=\langle n|\{a_\beta^{\dagger},a_\alpha\}|n\rangle, \tag{85}$$

we do, indeed, discover a different normalization,

$$|A_i(n)|^2=1-\sum_{jn'}|\eta_{ji}(n')|^2-\sum_j|\xi_{ji}(n)|^2, \tag{86}$$

the additional term following from the occurrence of the ground state as an intermediate state in the spectral decomposition of (85). We again find compatibility with the condition (54),

$$N=\sum_\alpha \langle n|a_\alpha^{\dagger}a_\alpha|n\rangle. \tag{87}$$

Finally, it is easy to check that off-diagonal elements of (54) consistently vanish.

We have thus exhausted the consequences of (54) and (55) for our approximation. In particular, we have obtained, in (81) and (86), renormalization of the HF amplitudes. We have yet to deduce any information, however, concerning the normalization of solutions of (66) and (67). As we shall now see, this will be determined by the self-consistency requirement,

$$\begin{aligned}W_N(0)+E(n)=&(\alpha|T|\alpha')\sum_{im}\psi_{im}(\alpha' m)\psi_{im}^*(\alpha n)\\ &+\tfrac{1}{2}(\alpha\beta|V|\alpha'\beta')\sum_{m'}[\sum_{j'm'}\psi_{i'm'}(\beta' n)\psi_{i'm'}^*(\beta n')]\\ &\times[\sum_{im}\psi_{im}(\alpha' n')\psi_{im}^*(\alpha n)].\end{aligned} \tag{88}$$

We consider first the case $n=0$, and write

$$W_N(0)=W_N^{(0)}(0)+\Delta W, \tag{89}$$

where $W_N^{(0)}(0)$ is the energy given by the HFA. For ΔW we obtain from (88) after some calculation in which account is taken of (64)–(67) and (81)

$$\begin{aligned}\Delta W&=\tfrac{1}{2}\sum_{nji}\{E(n)-[\mathcal{E}_j-\mathcal{E}_i]\}[|\xi_{ji}(n)|^2-|\eta_{ji}(n)|^2]\\ &=\sum_n \Delta W(n).\end{aligned} \tag{90}$$

The corresponding calculation for an excited state, which employs the same equations as needed for (90), and (86) in addition, yields, after some algebra,

$$\begin{aligned}W_N(0)+E(n)=&W_N^{(0)}(0)+\Delta W-\Delta W(n)\\ &+E(n)\sum_{ji}\{|\xi_{ji}(n)|^2-|\eta_{ji}(n)|^2\}.\end{aligned} \tag{91}$$

We make use of (89) and conclude that self-consistency here yields a normalization condition appropriate to

the positive energy eigenvalues,

$$|f(n)|^2 \equiv \sum_{ji} \{|\xi_{ji}(n)|^2 - \eta_{ji}(n)|^2\} = 1 + [\Delta W(n)/E(n)]. \quad (92)$$

If we renormalize $\xi_{ji}(n)$ and $\eta_{ji}(n)$ so that

$$\sum_{ji} \{|\xi_{ji}^{(0)}(n)|^2 - |\eta_{ji}^{(0)}(n)|^2\} = 1, \quad (93)$$

then (92) and (90) imply

$$|f(n)|^2 = E(n)/[E(n) - \Delta W^{(0)}(n)], \quad (94)$$

where

$$\Delta W^{(0)}(n) = \tfrac{1}{2} \sum_{ji} [E(n) - (\mathcal{E}_j - \mathcal{E}_i)] \times \{|\xi_{ji}^{(0)}(n)|^2 - |\eta_{ji}^{(0)}(n)|^2\}. \quad (95)$$

The deviation of $f(n)$ from unity is a measure of the breakdown of the usual quasiboson picture attached to the RPA. Examination of Eqs. (94) and (95) indicates that such deviations may be the more appreciable, the smaller the excitation energy $E(n)$.

We have now completed our account of the fresh insights offered into the RPA from the vantage point of the GHFA. We conclude this section with a brief resume of some of the salient properties of the eigenvalue problem (66) and (67). This is best carried out after the introduction of a compact matrix notation for these equations.

In view of their structure, it appears natural to associate $\eta_{ji}^*(n)$ with $\xi_{ji}(n)$ as a vector. Indeed, we recognize the matrix $\mathbf{M}$ which plays a role in the stability considerations of Thouless,[15] (Appendix A). Defining the column vector $\mathbf{Z}(n)$,

$$Z_{ji}(n) = \begin{pmatrix} \xi_{ji}(n) \\ \eta_{ji}^*(n) \end{pmatrix}, \quad (96)$$

and the metric tensor τ_3, the third Pauli matrix, our equations may be written

$$\mathbf{M}\mathbf{Z}(n) = E(n)\tau_3\mathbf{Z}(n) \quad (97)$$

or

$$(\tau_3\mathbf{M})Z(n) = E(n)\mathbf{Z}(n). \quad (98)$$

It will be of consequence for what follows that the matrix $\tau_3\mathbf{M}$ is *not* Hermitian (although $\mathbf{M}$ is).

Let us briefly catalog some of the properties of (97). We first note that if $E(n)$ is a solution belonging to the eigenvector $\mathbf{Z}(n)$, then (allowing complex solutions) $-E(n)^*$ is also a solution with eigenvector

$$\tau_1\mathbf{Z}^*(n) = \begin{pmatrix} \eta \\ \xi^* \end{pmatrix}. \quad (99)$$

This follows from the property of $\mathbf{M}$ expressed by the equation

$$\tau_1\mathbf{M}\tau_1 = \mathbf{M}^*. \quad (100)$$

For physical consistency, we must, however, demand real eigenvalues $E(n)$. In the latter case there will be two sets, the positive eigenvalues $|E(n)|$ corresponding to the equations (66) and (67) as written, i.e., to the collective excitation energies of the N-particle system. The negative set $-|E(n)|$ are, in the present context, equally physical, since they correspond to the negative of the collective state energies of the $N-1$ particle system. Whereas (66) was obtained by studying the equations satisfied by the $\psi_{i0}(\alpha n)$, if we had instead studied the equations for the $\psi_{in}(\alpha 0)$, we should have obtained precisely the equations for the second set of solutions with the physical interpretation as given.

The necessary and sufficient condition that the $E(n)$ be real and nonzero is that $\mathbf{M}$ be positive definite. This is the same as the condition that the original HF solution be stable against small deformation.[15] The sufficiency condition is simple to prove: We study the expression

$$\mathbf{Z}^\dagger(n)\mathbf{M}\mathbf{Z}(n) = E(n)\mathbf{Z}^\dagger(n)\tau_3\mathbf{Z}(n) > 0, \quad (101)$$

i.e., since $\mathbf{M}$ is Hermitian and positive-definite the left-hand side is real and positive. Since $\mathbf{Z}^\dagger(n)\tau_3\mathbf{Z}(n)$ is also real, $E(n)$ must be real and of the same sign as the scalar product.

The converse takes the following form. If the $E(n)$ are real and nonzero, and if, as we shall establish independently below, (a) the eigenvectors form a complete set, (b) the sign of the scalar product is that of $E(n)$, then M is positive definite. For if $\mathbf{Z}$ is an arbitrary vector, we may then expand

$$\mathbf{Z} = \sum_n B(n)\mathbf{Z}(n), \quad (102)$$

and using the mutual orthogonality of the $\mathbf{Z}(n)$, with the metric τ_3, which follows from (97), we have

$$\mathbf{Z}^\dagger\mathbf{M}\mathbf{Z} = \sum_n |B(n)|^2 E(n)\mathbf{Z}^\dagger(n)\tau_3\mathbf{Z}(n) > 0. \quad (103)$$

We thus have the result that the condition for stability of the original HF solution and the condition that the RPA yield physically acceptable results (real eigenvalues) are one and the same.

To complete the picture, we must thus prove hypotheses (a) and (b). For the details of the proof of (a), we refer to the work of Thouless.[24] (We assume, as does he, that we are dealing with a finite-dimensional vector space.) The basic element of the proof is the observation that if two vectors $\mathbf{Y}$ and $\mathbf{X}$ are orthogonal in the sense

$$\mathbf{X}^\dagger\tau_3\mathbf{Y} = 0, \quad (104)$$

they are linearly-independent unless one of them has norm zero (as do the vectors for eigenvalue zero). The proof can then be constructed in close analogy to that for an Hermitian matrix.

The case for point (b) has, in fact, already been made

[24] For a previous account, see D. J. Thouless, Nucl. Phys. **22**, 78 (1961), where the reader will find some of the results given at the end of this section.

in connection with the study of the self-consistency requirement. It is that $[f(n)]^2$, Eq. (94) be positive, which should be true as long as $E(n)>0$.

A study of the problem of $E(n)=0$ is reserved for Appendix C.

V. THE GHFA APPLIED TO UNIFORM TRANSLATIONAL MOTION

In this section, we study the example for which the GHFA can be solved in all essentials exactly, i.e., the example in which we take into account the class of excited states which represent the ground state in uniform translational motion[25] with momentum K. We deal with one-dimensional motion, since this changes none of the important features of the problem. We work, conveniently, in coordinate space,

$$(\alpha|T|\beta)\rightarrow T(x,x')=\delta(x-x')(-\nabla^2/2m)$$
$$=\delta(x-x')(p^2/2m),$$
$$(\alpha\beta|V|\gamma\delta)\rightarrow V(x,x'';x,'x''').$$

We assume that V is both translationally invariant,

$$V(x+X,x''+X;x'+X,x'''+X)=V(x,x'';x',x'''),\quad(105)$$

and Galilean invariant,

$$V(x,x'';x',x''')=\delta(x+x''-x'-x''')\times v(x,x'';x',x'''). \quad (106)$$

The fundamental equations to be solved self consistently fall into several categories. The modes which describe a generalized hole in the N-particle systems satisfy

$$[\mathcal{E}_{iQ}+E(K)]\psi_{iQ}(xK)=(p^2/2m)\psi_{iQ}(xK)+(xK|\mathcal{U}|x'K')\psi_{iQ}(x'K'),\quad(107)$$

$$(xK|\mathcal{U}|x'K')=V(x,x'';x',x''')(x'''K|\rho|x''K'),\quad(108)$$

$$(xK|\rho|x'K')=\textstyle\sum_{iQ}\psi_{iQ}(xK)\psi_{iQ}^*(x'K'),\quad(109)$$

and

$$\int dx(xK|\rho|xK')=N\delta_{KK'}.\quad(110)$$

We must simultaneously consider the generalized particle modes satisfying

$$[\mathcal{E}_{jQ}-E(K)]\phi_{jQ}(xK)=(p^2/2m)\phi_{jQ}(xK)+(xK'|\mathcal{U}|x'K)\phi_{jQ}(x'K'),\quad(111)$$

since the two sets are coupled by the condition

$$(xK|\rho|x'K')+(xK|\tau|x'K')=\delta(x-x')\delta_{KK'},\quad(112)$$

with

$$(xK|\tau|x'K')=\sum_{jQ}\phi_{jQ}(xK')\phi_{jQ}^*(x'K).\quad(113)$$

[25] The problem studied in this section has also been investigated by a method whose spirit is similar to ours by M. Bolsterlei, Phys. Rev. **129**, 2830 (1963).

Finally we have the self-consistency condition

$$W_N(0)+E(K)=W_N(0)+(K^2/2M)=T(x,x')(x'K|\rho|xK)+\tfrac{1}{2}V(x,x'';x',x''')(x'''K|\rho|x''K')\times(x'K'|\rho|xK).\quad(114)$$

We first show in what sense (107)–(110) can be solved exactly for the given spectrum $E(K)$, i.e., the given "total mass" M. We shall then examine the extent to which the remaining conditions can be satisfied. It is convenient first to transform these equations by introducing a complete set of localized states,

$$|X\rangle=|K\rangle\langle K|X\rangle=L^{-1/2}\exp(-iKX)|K\rangle,$$
$$\langle X|X'\rangle=\delta(X-X'),\quad(115)$$

where L is the size of the system. If $P_{\rm op}$ is the total momentum operator of the actual physical system we have

$$\exp(iP_{\rm op}X)|X\rangle=|X=0\rangle,\quad(116)$$

with the definition

$$\psi_{iQ}(xX)=\psi_{iQ}(xK)\langle K|X\rangle,\quad(117)$$

Eq. (107) transforms to

$$[\mathcal{E}_{iQ}-(\partial^2/2M\partial X^2)]\psi_{iQ}(xX)=(p^2/2m)\psi_{iQ}(xX)+(xX|\mathcal{U}|x'X')\psi_{iQ}(x'X').\quad(118)$$

If $\psi(x)$ is the destruction operator at the point x, we have, using the translational invariance in all its meanings

$$\psi_{iQ}(xX)=\langle iQ|\psi(x)|X\rangle=\langle iQ|\psi(x)\exp(-iP_{\rm op}X)|X=0\rangle=\langle iQ|\exp(-iP_{\rm op}X)\psi(x-X)|X=0\rangle\equiv L^{-1/2}\exp(-iQX)f_{iQ}(x-X),\quad(119)$$

where we have thus chosen $|iQ\rangle$ to be an eigenstate of total momentum with eigenvalue Q, and we have defined the amplitude $f_{iQ}(x)$.

We find upon insertion of (119) into (118) and with the help of the definitions

$$\mathcal{E}_i+\delta\mathcal{E}_{iQ}=\mathcal{E}_{iQ}+Q^2/2M,\quad(120)$$

$$\mu=mM/(M-m),\quad(121)$$

that

$$[\mathcal{E}_i+\delta\mathcal{E}_{iQ}+(Qp/M)-(p^2/2\mu)]f_{iQ}(x-X)=\exp[iQ(X-X')](xX|\mathcal{U}|c'X')f_{iQ}(x'-X').\quad(122)$$

The combination

$$-(p^2/2\mu)+(Qp/M)=-(1/2\mu)[p-(\mu Q/M)]^2+(\mu Q^2/2M^2)\quad(123)$$

suggests the substitution

$$f_{iQ}(x-X)=\exp[i(\mu Q/M)(x-X)]f_i(x-X),\quad(124)$$

and the identification

$$\delta\mathcal{E}_{iQ}=-\mu Q^2/2M^2.\quad(125)$$

It remains to be shown, however, that the resulting equation,

$$[\mathcal{E}_i-p^2/2\mu]f_i(x-X) = \exp\{-i(\mu Q/M)(x-X-x'+X')+iQ(X-X')\} \times(xX|\mathcal{U}|x'X')f_i(x'-X'), \quad (126)$$

is, in fact, independent of Q, so that (124) and (125) represent a self-consistent possibility.

Toward this end we study the density matrix

$$\begin{aligned}(xX|\rho|x'X') &= \sum_{iQ}\psi_{iQ}(xX)\psi_{iQ}^*(x'X') \\ &= \sum_i \delta\{(X-X')[1+(\mu/M)]-(x-x')(\mu/M)\} \\ &\quad\times f_i(x-X)f_i^*(x'-X') \\ &= (M/M+\mu)\delta[(X-X')+(x-x')(\mu/M+\mu)] \\ &\quad\times\sum_i f_i(x-X)f_i^*[x'-X+(x-x') \\ &\quad\times(\mu/M+\mu)], \quad (127)\end{aligned}$$

which has been evaluated with the help of (119) and (124). If we remember the condition for Galilean invariance, Eq. (124), and substitute (127) into (126), we find that the phase factors dependent on Q cancel and we end up with the equation

$$\begin{aligned}[\mathcal{E}_i-(p^2/2\mu)]f_i(x-X) &= (M/M+\mu)V(x,x'';x',x''') \\ &\quad\times\{\sum_{i'} f_{i'}(x'''-X) \\ &\quad\times f_{i'}^*[x''-X+(x-x')(\mu/M+\mu)]\} \\ &\quad\times f_i[x'-X+(x-x')(\mu/M+\mu)]. \quad (128)\end{aligned}$$

From the translational invariance of V, we see that the solutions of (128) do not depend on the precise value of X. Setting $X=0$ and carrying out a simple change of variables, we may write

$$[\mathcal{E}_i-(p^2/2\mu)]f_i(x)=\mathcal{U}[x,x';(\mu/M)]f_i(x'), \quad (129)$$

where

$$\mathcal{U}[x,x';(\mu/M)] = V[x,x''+(x'-x)(\mu/M);x'+(x'-x)(\mu/M),x'''] \times\sum_i f_i(x''')f_i^*(x''). \quad (130)$$

It is easy to see that $\mathcal{U}[x,x';(\mu/M)]$ is Hermitian and as $(\mu/M)\to 0$, it reduces to the customary HF potential. Presuming that (129, 130) can be solved self consistently we have for a *given* mass M found the exact solutions to (107)–(109).

In order actually to find the solution of (129), we must know what norm to assign to the $f_i(x)$, assuming from the known HF limit that we must choose precisely N solutions. A complete answer to this question involves necessarily the simultaneous study of (110)–(113). Here we shall infer the result from (110) alone and show the self consistency of (114) before carrying out a more formally complete study. From (127) we find

$$\begin{aligned}N\delta(X-X') &= \int dx(xX|\rho|xX') \\ &= \delta(X-X')[M/(M+\mu)]\sum_i \|f_i\|^2, \quad (131)\end{aligned}$$

and thus infer, assigning equal norm to each mode, that

$$\|f_i\|^2=(M+\mu)/M. \quad (132)$$

The self-consistency condition now yields, with the aid of (127), (130), and (132)

$$\begin{aligned}W_N(0) &= (M/M+\mu)^2\sum_i\int f_i^*(x)(p^2/2\mu)f_i(x) \\ &\quad+\tfrac{1}{2}(M/M+\mu)\int V[x,x';(\mu/M)] \\ &\quad\times[\sum_i f_i(x')f_i^*(x)], \quad (133)\end{aligned}$$

$$\begin{aligned}(K^2/2M) &= \sum_i \|f_i\|^2[M\mu^2/(M+\mu)^3](K^2/2m) \\ &= (Nm/M)(K^2/2M)[1+O(m/M)]. \quad (134)\end{aligned}$$

From (133) we see that the ground-state energy is essentially that given by the HF theory except for corrections of relative order N^{-1}, whereas from (134) we find the result which helps substantiate the soundness of our method, namely $M=Nm$, again with corrections of relative order N^{-1}.

As a final point, it is not difficult to verify that our solution (127) for the density matrix confirms the input hypothesis of the method, in that a study, for example, of matrix elements such as $(xK|\rho|x'K')$, $K\neq K'$, shows that they are sensibly the same order of magnitude as the diagonal elements $K=K'$ as long as $|K-K'|\lesssim R^{-1}$, where R is the size of the single-particle functions.

In the application of our method to physically more interesting problems of collective motion, where the exact solutions are not known, it will be necessary to resort to an approximation method to obtain self-consistent solutions to the desired accuracy. It will, therefore, prove instructive to develop this method first for the example at hand. Incidentally, we shall verify to the required order that we can also solve Eqs. (111) and (112), which we have so far ignored.

We, therefore, study (107) and (111) following a procedure suggested by the investigations of the previous section. We can unify and simplify our considerations of these two equations if we are willing to replace μ, Eq. (121), by m and similarly for the corresponding quantity $\mu'=[Mm/(M+m)]$ which can be shown to enter in the study of (111). With this approximation,

and with the definition (119) and

$$\phi_{jQ}(x,X)=L^{-1/2}e^{iQX}f_{jQ}(x-X), \tag{135}$$

the two equations to be considered are the following approximations to (122),

$$[\mathcal{E}_i+(Qp/M)-(p^2/2m)]f_{iQ}(x-X) =\exp[iQ(X-X')](xX|\mathcal{U}|x'X')f_{iQ}(x'-X'), \tag{136}$$

and corresponding to (111) and (135)

$$[\mathcal{E}_j+(Qp/M)-(p^2/2m)]f_{jQ}(x-X) =\exp[-iQ(X-X')](xX'|\mathcal{U}|x'X) \times f_{jQ}(x'-X'). \tag{137}$$

Here we have dropped terms $\delta\mathcal{E}_{iQ}$ and $\delta\mathcal{E}_{jQ}$ because we shall use (136) and (137) only for the first-order change in the wave function about its HF value.

To solve (136), for example, we try

$$f_{iQ}(x)=f_i(x)+\sum_{a\neq i} f_a(x)C_{ai}(Q). \tag{138}$$

We emphasize that (138) is correct to first order only. Second-order corrections will be discussed briefly below. From (136) and (138) we find

$$\begin{aligned}(a|p|i)(Q/M)=&(\mathcal{E}_a-\mathcal{E}_i)C_{ai}(Q)\\ &+\int dxdx'dx''dx'''dX'f_a^*(x-X)\\ &\times\exp[iQ(X-X')]V(x,x'';x',x''')\\ &\times\sum_{a'i'K}L^{-1}\exp[-iK(X-X')]\\ &\times\{f_{a'}(x'''-X)f_{i'}^*(x''-X')C_{a'i'}(K)\\ &+f_{i'}(x'''-X)f_{a'}^*(x''-X')C_{a'i'}^*(K)\}\\ &\times f_i(x'-X'). \end{aligned}\tag{139}$$

This equation can be simplified if we follow the suggestion contained in the inhomogeneous term and assume that

$$C_{ai}(Q)=(Q/M)c_{ai}. \tag{140}$$

Upon introduction of (140) into (139) and integration by parts we obtain

$$(a|p|i)=(\mathcal{E}_a-\mathcal{E}_i)c_{ai}+(ai'|V|ia')c_{a'i'} +(aa'|V|ji')c_{a'i'}. \tag{141}$$

To reach the form (141) we have been forced to discard several terms which vanish if we assume parity conservation.

Several interesting consequences can be drawn immediately from (141). By studying the equation with $a=i$ and then that obtained by interchanging i and i', we learn that

$$c_{i'i'}=-c_{ii'}^*. \tag{142}$$

Equation (142) is sufficient to cause terms depending on these coefficients in the equation for $a=j$ to cancel. Thus, the equations for the quantities c_{ji} and c_{ji}^* are closed and we can consistently set $c_{i'i}=0$. That we are *required* to do so in this approximation follows from reasoning similar to that associated with Eq. (76) of the previous section.

Similarly, we can solve (137) by assuming

$$f_{jQ}(x)=f_j(x)+\sum_i f_i(x)C_{ij}(Q/M), \tag{143}$$

where we have already incorporated the analog of (140) and (142). The resulting equation for C_{ij}, not to be recorded, demonstrates that

$$C_{ij}=-C_{ji}^*. \tag{144}$$

We are thus left with the necessity of solving the simplified form of (141), which together with its complex conjugate can be written in matrix form,

$$\mathbf{p}=\mathbf{MC}, \tag{145}$$

where

$$(j|\mathbf{p}|i)=\begin{pmatrix}(j|p|i)\\(j|p|i)^*\end{pmatrix},\quad \mathbf{C}_{ji}=\begin{pmatrix}C_{ji}\\C_{ji}^*\end{pmatrix}, \tag{146}$$

and M is the familiar matrix encountered both in the study of stability of HF solutions and of the RPA.

We verify that (145) admits the solution

$$C_{ji}=im(j|x|i). \tag{147}$$

For this purpose we use the assumption that x commutes with the interaction V, since the latter has been supposed Galilean invariant. The lemma of Appendix C then tells us that (145) may be written in the form

$$\begin{aligned}(j|p|i)&=-(j|[C,\mathcal{H}]|i)+(j|[C,\mathcal{U}]|i)\\ &=-im(j|[x,(p^2/2m)]|i),\end{aligned} \tag{148}$$

which is, indeed, an identity. The importance of the terms depending on the potential in reaching this result is evident: These terms take account of the nonlocality or velocity dependence of the self-consistent potential. It is also clear that displacing x in (147) by any constant does not alter any of our considerations so that the result coincides precisely to first order with the exact solution, Eq. (124).

The reader will note that to this point we have still taken no heed of the normalization condition (112). The first-order solution defined by (138) and (140) is, however, not sufficiently accurate for use in the self-consistency condition (114), since it is not difficult to see that an alteration in the norm of the solution which is of second order in (Q/M) will contribute to the total mass. If we restrict ourselves to the limit in which $(m/M)\to 0$, (Q/M) remaining finite, we can write to

second order in the latter quantity

$$f_{iQ}(x)=A_i(Q)f_i(x)+\sum_j f_j(x)C_{ji}(Q/M)+\sum_{a\neq i} f_a(x)d_{ai}(Q/M)^2+\cdots, \quad (149)$$

$$f_{2Q}(x)=A_j(Q)f_j(x)+\sum_i f_i(x)C_{ij}(Q/M)+\sum_{a\neq j} f_a(x)d_{aj}(Q/M)^2+\cdots. \quad (150)$$

Here $A_i(Q)$ and $A_j(Q)$ are normalization constants, the f_a being supposed a complete orthonormal set; by inserting (149) and (150) in (119) and (135), respectively, and the latter into (112), we can deduce the values of $A_i(Q)$ and $A_j(Q)$. (The nondiagonal second-order terms d_{ai}, d_{aj} were included above only to illustrate the form of the expansion.) We find

$$|A_i(Q)|^2=1-\textstyle\sum_j |C_{ij}|^2(Q/M)^2, \quad (151)$$

$$|A_j(Q)|^2=1-\textstyle\sum_i |C_{ji}|^2(Q/M)^2. \quad (152)$$

It is essential to emphasize that the change in normalization of the hole modes arises according to (150) and (151) from the first-order corrections to the particle modes and conversely from (149) and (152). Nevertheless, in virtue of Eq. (144) the result we have found in (151) and (152) is here tantamount to the requirements (to second order at least) that the wave functions $\psi_{iQ}(xX)$, $\phi_{jQ}(xX)$ be each normalized according to

$$\int dxdX\ |\psi_{iQ}(x,X)|^2=\int dxdX\ |\phi_{jQ}(x,X)|^2=1. \quad (153)$$

The corresponding conclusion was not applicable in the study of the RPA.

We leave as an assertion that with the corrected normalization (151), we can, from the self-consisting requirement (114) derive anew the correct value of the mass.

It is worth pointing out finally that in the semiclassical limit in which we are now working a simplified derivation of a formula for the collective parameter M can be given. In this limit of $(m/M)\to 0$, the ground-state energy is independent of the value of M, and we can proceed therefore by means of the formula

$$\int_0^{M^{-1}} dM^{-1}(\partial/\partial M^{-1})\sum_K W_N(K)=\sum_K (K^2/2M). \quad (154)$$

Though (154) holds for each K, the result we seek is obtained more easily by making use of the properties of the trace. Applying (154) to (114), making use of (107) and of the assumed normalization condition

$$(\partial/\partial M^{-1})\int dx\sum_K \psi_{iQ}^*(xK)\psi_{iQ}(xK)=0, \quad (155)$$

we obtain after some calculation

$$\sum_Q (Q^2/2M)=\frac{1}{2}\int dxdX \times\sum_{iQ}\{\delta\psi_{iQ}^*(xX)(pQ/M)\psi_{iQ}(xX)+\psi_{iQ}^*(xX)(pQ/M)\delta\psi_{iQ}(xX)\}, \quad (156)$$

where

$$\delta\psi_{iQ}(xX)=L^{-1/2}\exp(-iQX)f_j(x-X)(Q/M)C_{ji}. \quad (157)$$

From (156) and (157), we find directly that

$$M=\textstyle\sum_{ij} C_{ji}^*(j|p|i)+C_{ji}(j|p|i)^* =\sum_i -im(i|[x,p]|i)=Nm. \quad (158)$$

The main point, however, is that we shall find that formulas like (158) will be useful in the future applications of the GHFA.

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APPENDIX A: STABILITY CONDITIONS IN THE HARTREE-FOCK APPROXIMATION

As an application of the results in Sec. II we study the condition [1,15] that the solutions ψ_i yield a true local minimum of the energy. In the expression (36), which is a functional $W[\psi_i^\dagger,\psi_i]$, we replace

$$\psi_i\to\psi_i'=\psi_i+\delta\psi_i, \quad (A1)$$

where the ψ_i' constitute a different orthonormal set, so that for instance

$$\|\psi_i'\|^2=1=1+(\psi_i,\delta\psi_i)+(\delta\psi_i,\psi_i)+(\delta\psi_i,\delta\psi_i). \quad (A2)$$

We find by straightforward calculation to second order in $\delta\psi_i$

$$\Delta W=W[\psi_i',\psi_i'^\dagger]-W[\psi_i,\psi_i^\dagger]=-\mathrm{tr}\sum_{i=1}^N \mathcal{E}_i\delta\psi_i\delta\psi_i^\dagger+\mathrm{tr}(T+\mathcal{U})\sum_i \delta\psi_i\delta\psi_i^\dagger+\mathrm{tr}\tfrac{1}{2}V[\sum_i(\delta\psi_i\psi_i^\dagger+\psi_i\delta\psi_i^\dagger)]\times[\sum_{i'}(\delta\psi_{i'}\psi_{i'}^\dagger+\psi_{i'}\delta\psi_{i'}^\dagger)], \quad (A3)$$

in which the first term was obtained with the aid of (27), (6), and (A2). The condition that the ψ_i' also

represent a set of orthonormal vectors within the N-dimensional subspace defined by the ψ_i permits us to write

$$\delta\psi_i=\sum_{i'=1}^{N}\psi_{i'}x_{i'i}+\sum_j\psi_j x_{ji}, \tag{A4}$$

where $x_{i'i}{}^*=-x_{ii'}$, but no condition other than smallness is thereby imposed on the x_{ji}. But the first term of (A4) represents a unitary transformation within the subspace of the ψ_i and, as is readily verified, leaves ρ and, therefore, the value of the energy unchanged. We may therefore simplify (A4) to

$$\delta\psi_i=\psi_j x_{ji}, \tag{A5}$$

where the sum is over unoccupied levels only. One can check directly that (30) and (31) are satisfied to first order.

With the help of (42) and (27), Eq. (40) now becomes

$$\Delta W=\sum_{i,j}(\mathcal{E}_j-\mathcal{E}_i)|x_{ji}|^2+\tfrac{1}{2}(ii'|V|jj')x_{ji}x_{j'i'}+\tfrac{1}{2}(ij'|V|ji')x_{ji}x_{j'i'}{}^*+\tfrac{1}{2}(ji'|V|ij')x_{ji}{}^*x_{j'i'}+\tfrac{1}{2}(jj'|V|ii')x_{ji}{}^*x_{j'i'}{}^*, \tag{A6}$$

where

$$(ab|V|cd)=(\alpha\beta|V|\gamma\delta)\psi_a{}^*(\alpha)\psi_b{}^*(\beta)\psi_c(\gamma)\psi_d(\delta). \tag{A7}$$

The content of (A6) may be rendered manifest by writing it in the form

$$\Delta W=\tfrac{1}{2}(X^\dagger)_{ji}M_{ji;j'i'}X_{j'i'}=\tfrac{1}{2}\mathbf{X}^\dagger\mathbf{M}\mathbf{X}, \tag{A8}$$

where

$$X_{ji}=\begin{pmatrix}x_{ji}\\ x_{ji}{}^*\end{pmatrix}, \tag{A9}$$

and

$$M_{ji;j'i'}=\begin{pmatrix}(\mathcal{E}_j-\mathcal{E}_i)\delta_{jj'}\delta_{ii'}+(ji'|V|ij') & (jj'|V|ii')\\ (ii'|V|jj') & (\mathcal{E}_j-\mathcal{E}_i)\delta_{jj'}\delta_{ii'}+(ij'|V|ji')\end{pmatrix}. \tag{A10}$$

Since $\mathbf{M}$ is Hermitian, we introduce its eigenvectors

$$\mathbf{M}\mathbf{X}(\omega)=\omega\mathbf{X}(\omega), \tag{A11}$$

and expanding our arbitrary vector $\mathbf{X}$,

$$\mathbf{X}=\textstyle\sum_\omega c(\omega)\mathbf{X}(\omega), \tag{A12}$$

obtain

$$\Delta W=\tfrac{1}{2}\textstyle\sum_\omega|c(w)|^2\omega. \tag{A13}$$

Thus, the condition for a local minimum is that all the eigenvalues of the matrix $\mathbf{M}$ be positive. The relationship of this condition to the excited states of the system, as computed in the RPA is explored in detail in Sec. IV. Several interesting discussions of stability questions for particular systems have been given recently.[1,26–28]

As a second application of these ideas, we ask, within the HF framework for the change in energy of the system due to a small change in the Hamiltonian,

$$T\rightarrow T+\delta T,\quad V\rightarrow V+\delta V. \tag{A14}$$

If $\rho^{(0)}$ is the unperturbed density matrix, then to first order we find trivially by means of the HF factorization

$$\delta_1 W=\mathrm{tr}\delta T\rho^{(0)}+\tfrac{1}{2}\,\mathrm{tr}\delta V\rho^{(0)}\rho^{(0)}=\sum_i(i|\delta T|i)+\tfrac{1}{2}\sum_{ii'}(ii'|V|ii'). \tag{A15}$$

We shall be more interested in the case where one has to go to second order. If we write

$$\delta\psi_i=\psi_j f_{ji}, \tag{A16}$$

and we define a matrix $\mathbf{F}$ as in (A9), we find by the same reasoning as led to (A8)

$$\delta_2 W=\tfrac{1}{2}\mathbf{F}^\dagger\mathbf{M}\mathbf{F}+\mathbf{F}^\dagger\delta\mathbf{T}+\mathbf{F}^\dagger\delta V, \tag{A17}$$

where, e.g.,

$$(j|\delta\mathbf{V}|i)=\begin{pmatrix}(j|\delta\mathcal{U}|i)\\ (j|\delta\mathcal{U}|i)^*\end{pmatrix}, \tag{A18}$$

and

$$(j|\delta\mathcal{U}|i)=(\alpha\beta|\delta V|\gamma\delta)\psi_j{}^*(\alpha)\psi_i(\gamma)\times[\sum_{i'}\psi_{i'}(\delta)\psi_{i'}{}^*(\beta)]. \tag{A19}$$

The result (A17) may be simplified, since from Eq. (27) and its complex conjugate we can derive the equation

$$\mathbf{M}\mathbf{F}=-\delta\mathbf{T}-\delta V, \tag{A20}$$

which permits (A17) to take the simpler form

$$\delta_2 W=\tfrac{1}{2}\mathbf{F}^\dagger(\delta\mathbf{T}+\delta V)=-\tfrac{1}{2}\mathbf{F}^\dagger\mathbf{M}\mathbf{F}. \tag{A21}$$

To evaluate (A21) we require the solution of (A20) which in general will be given in terms of the eigenvectors of $\mathbf{M}$.

If we once more expand in the set $\mathbf{X}(\omega)$ we have

$$\delta_2 W=-\tfrac{1}{2}\textstyle\sum_\omega\omega|f(\omega)|^2, \tag{A22}$$

where

$$\mathbf{F}=\textstyle\sum_\omega f(\omega)\mathbf{X}(\omega). \tag{A23}$$

Inserting this into (A20) and expanding

$$\delta\mathbf{T}+\delta V\equiv\delta\mathcal{H}=\textstyle\sum_\omega\delta h(\omega)\mathbf{X}(\omega), \tag{A24}$$

we have

$$f(\omega)=\delta h(\omega)/\omega\quad\text{when}\quad\omega\neq0, \tag{A25}$$

and then

$$\delta_2 W=-\tfrac{1}{2}\textstyle\sum_\omega|\delta h(w)|^2/w, \tag{A26}$$

[26] I. Ia Pomeranchuk, Zh. Eksperim. i Teor. Fiz. **35**, 524 (1958) [translation: Soviet Phys.—JETP **8**, 361 (1959)].
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which reduces to second-order perturbation theory if the eigensolutions $\mathbf{X}(\omega)$ of (A20) are calculated neglecting the matrix elements of V in (A10).

APPENDIX B: A VARIATIONAL APPROACH TO THE GENERALIZED HARTREE-FOCK APPROXIMATION

A possible variational formulation for the GHFA may be stated as follows: The GHFA method is equivalent to the requirement

$$\delta \sum_n \langle n|H|n\rangle = 0\,, \tag{B1}$$

where $\langle n|H|n\rangle$ is given by Eq. (60) and the $\psi_i(\alpha n)$, $\psi_i^*(\alpha n)$ are to be varied, subject to the constraints

$$\delta \sum_{\alpha,i} \psi_i(\alpha n)\psi_i^*(\alpha n) = \delta N = 0\,, \tag{B2}$$

which is a special case of (54), and to a normalization condition

$$\delta \sum_{\alpha n} \psi_i(\alpha n)\psi_i^*(\alpha n) = \delta 1 = 0\,. \tag{B3}$$

Using the method of Lagrange multipliers we have

$$\delta \sum_n \{\langle n|H|n\rangle - \sum_{\alpha,i} (E(n)+\mathcal{E}_i)\psi_i(\alpha n)\psi_i^*(\alpha n)\} = 0\,, \tag{B4}$$

$E(n)$ serving as Lagrange multiplier for the condition (B2), $\mathcal{E}_i$ for the condition (B3). Equation (B4) is formally equivalent to (48).

It appears, however, that the variational formulation is incomplete. To understand this assertion, let us consider first the usual HFA. In that case, the derivation based on the equations of motion provides from the start the physical interpretation of the parameters $\mathcal{E}_i$ as energy differences. In the variational formulation the $\mathcal{E}_i$ appear initially as Lagrange multipliers. Their physical significance is established as follows: From the density matrix $\rho \equiv \rho(N,0)$,

$$\rho(N,0) = \sum_{i=1}^{N} \psi_i \psi_i^\dagger\,, \tag{B5}$$

we calculate $W_N(0)$. From the physical interpretation of $\rho(N,0)$ and of the ψ_i, we conclude that we may calculate the energies $W_{N-1}(i)$ from the HF formula using density matrices

$$\rho(N-1,i) = \sum_{i' \neq i} \psi_{i'} \psi_{i'}^\dagger\,. \tag{B6}$$

We then find up to relative order N^{-1},

$$\begin{aligned} W_N(0) - W_{N-1}(i) &= \psi_i^*(\alpha)(\alpha|\mathcal{H}|\beta)\psi_i(\beta) \\ &= \mathcal{E}_i\,, \end{aligned} \tag{B7}$$

the latter equality being derived from the HF equations themselves.

The corresponding relationship for the GHFA contains less information. In order to obtain it, we suggest the following interpretation of our theory. Just as we have introduced the "band" of excited states associated with the ground state of the N-particle system, so have we also supposed that the index i of the $N-1$ particle system is somewhat more explicitly written as im, where i indicates one of the intrinsic states and m is a member of the "band" associated with it. For each i, there are presumed to be η values of m. As a special case of (54) or (B2), we have, for example,

$$\sum_{\alpha m i} \psi_{im}(\alpha n)\psi_{im}^*(\alpha n) = N\,. \tag{B8}$$

We must now recognize the essential new element of the GHFA. Whereas before a density matrix was associated with a given state of our system, it is now associated with a band of states. Thus, the analog of (B5) is

$$\rho(N,0) = \sum_{im} \psi_{im} \psi_{im}^\dagger\,, \tag{B9}$$

and of (B6)

$$\rho(N-1,i') = \sum_{i,m\,(i\neq i')} \psi_{im} \psi_{im}^\dagger\,. \tag{B10}$$

From these formulas and the conservation of particles we can suggest that (B8) may be replaced by

$$\sum_{\alpha m} \psi_{im}(\alpha n)\psi_{im}^*(\alpha n) = 1\,. \tag{B11}$$

With the help of (B11) and (B3), we find from the GHFA Eq. (48), that

$$\begin{aligned} \sum_m \mathcal{E}_{im} + \sum_n E(n) = \sum_{\alpha n,\alpha' n',m} & \psi_{im}^*(\alpha n)(\alpha n|\mathcal{H}|\alpha' n') \\ & \times \psi_{im}(\alpha' n')\,. \end{aligned} \tag{B12}$$

On the other hand, from the equations of motion, we should have

$$\begin{aligned} \sum_m \mathcal{E}_{im} + \sum_n E(n) = \sum_n W_N(n) \\ - \sum_m W_{N-1}(im)\,. \end{aligned} \tag{B13}$$

This is seen to be consistent with (B12) if we compute the first sum on the right-hand of (B13) from (60) with the help of (B9), the second sum analogously using (60) and (B10). The assignment of density matrices to the neighboring system of $N-1$ particles according to (B10) is thus seen to be consistent with the basic equations of the GHFA.

These considerations, however, and we know no other, are unable to establish the physical interpretation of the individual $\mathcal{E}_{im}$, $E(n)$. Since the latter especially is needed to complete the self-consistency, we must conclude, at least tentatively, that a fully equivalent variational formulation does not exist. On the other hand, an equivalent density-matrix formulation does exist. In this, Eq. (48) is replaced by the condition

$$[\rho,\mathcal{H}] = 0 \tag{B14}$$

in the enlarged space, the additional definitions and

requirements remaining the same. Equation (B14) is itself deduced directly from (48). This last formulation is the one outlined in Sec. I.

APPENDIX C: ZERO-FREQUENCY SOLUTIONS OF THE RANDOM-PHASE APPROXIMATION

We discuss here the physical meaning of the zero-energy solutions of the equations of the RPA. In this case we may restrict ourselves to solutions of the form

$$Z_{ji}(0)=\begin{pmatrix}\xi_{ji}\\ \xi_{ji}^*\end{pmatrix}, \tag{C1}$$

which necessarily have zero norm. Our equations then become identical to the equations which determine incipient instability of the HF solutions [Eqs. (A10) and (A11)] and are

$$(\mathcal{E}_i-\mathcal{E}_j)\xi_{ji}=(ji'|V|ij')\xi_{j'i'}+(jj'|V|ii')\xi_{j'i'}^*, \tag{C2}$$

and complex conjugate equation.

In the stability problem, we start with a complete set of orthonormal single-particle functions $\psi_a(\alpha)$, such that only the first N, $\psi_i(\alpha)$, determine the energy and compare a "neighboring" set $\psi_a'(\alpha)=\psi_a(\alpha)+\delta\psi_a(\alpha)$. The relation

$$\delta\psi_a(\alpha)=\psi_b(\alpha)\xi_{ba} \tag{C3}$$

must then constitute an infinitesimal unitary transformation, or

$$\xi_{ba}=-\xi_{ab}^*, \tag{C4}$$

a substitution that will, henceforth, be made in (C2). We, furthermore, define $\xi_{\rm op}$ as the operator

$$\xi_{\rm op}=a_\alpha^\dagger\xi_{\alpha\beta}a_\beta,$$
$$\xi_{\alpha\beta}=\psi_a(\alpha)\xi_{ab}\psi_b^*(\beta). \tag{C5}$$

We first establish the following basic lemma: If the commutator

$$[\xi_{\rm op},V_{\rm op}]=0, \tag{C6}$$

i.e., if the interaction is invariant under the unitary transformations generated by $\xi_{\rm op}$ then

$$(j|[\xi,\mathcal{V}]|i)=\xi_{j'i'}(ji'|V|ij')-(jj'|V|ii')\xi_{i'j'}. \tag{C7}$$

Proof: If we work out the commutator (C6), we must find that it implies and is implied by the statement

$$\xi_{\alpha\epsilon}(\epsilon\beta|V|\delta\tau)-(\alpha\beta|V|\epsilon\tau)\xi_{\epsilon\delta}=\xi_{\beta\epsilon}(\epsilon\alpha|V|\delta\tau)-(\alpha\beta|V|\epsilon\delta)\xi_{\epsilon\tau}. \tag{C8}$$

Converting to the complete set $\psi_a(\alpha)$, a special case of (C8) reads

$$\xi_{ja}(ai'|V|ii')-(ji'|V|ai')\xi_{ai}=\xi_{i'a}(aj|V|ii')-(ji'|V|ai)\xi_{ai'}. \tag{C9}$$

But the left-hand side of (C9) is by definition the left-hand side of (C7). The right-hand sides are also equal if we notice that their difference

$$\xi_{i''i'}(ji'|V|ii'')-(ji''|V|ii')\xi_{i'i''}\equiv 0. \tag{C10}$$

From the lemma given, now follows the theorem:

Theorem: If $\xi_{\rm op}$ also commutes with $T_{\rm op}$ so that

$$[\xi_{\rm op},T_{\rm op}]=[\xi_{\rm op},(T_{\rm op}+V_{\rm op})]=[\xi_{\rm op},H]=0, \tag{C11}$$

but ξ is *not* a constant of the motion of the HF Hamiltonian

$$[\xi,V]\neq 0, \tag{C12}$$

then ξ is a nontrivial solution of Eq. (C2). This follows from the fact that with the help of (C7) and (C11), we have now established that Eq. (C2) is equivalent to the identity

$$(\mathcal{E}_i-\mathcal{E}_j)\xi_{ji}=(j|[\xi,H]|i) \tag{C13}$$

and from (C12), we know that this identity is nontrivial.

Thus, for every one-particle symmetry operation of the original Hamiltonian which is violated by the HF Hamiltonian we obtain a zero-frequency solution of the RPA, which solution is formed from the matrix elements of the generator of the corresponding symmetry operation. The physical meaning of this result is well known from particular examples previously given.[22] Thus, in the case of the spherical nuclear shell model, where the original Hamiltonian is translationally invariant, but the HF wave functions are not eigenfunctions of momentum, but rather represent wave functions centered about a given origin, our result expresses the fact that the HF energy is unaltered by translating this origin. We thus have three independent zero-energy solutions. Similarly, in the case of the spheroidal shell model, the arbitrariness in the choice of orientation of the well yields two more zero-energy solutions corresponding to the independent rotations about axes perpendicular to the axis of symmetry.

As we have seen in Sec. V on the example of translation, the GHFA is precisely the tool which yields a deeper understanding of how it is that a state of definite symmetry is best represented in the HFA by a Slater determinant which violates that symmetry.