Self-Consistent Theory of Nuclear Spectra: Pairing-Force Model*

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In prior work, we have studied the pairing interaction by means of the equations of motion satisfied by the matrix elements of single-fermion operators (coefficients of fractional parentage). The previous numerical calculations incorporated approximations which we seek to avoid here by developing a self-consistent theory fully consonant with the intrinsic structure of the equations of motion and associated conditions. Unlike other methods, where a distinction is usually made between the ground state and other low-lying excited states, we here consider the subspace defined by all these states on an equal footing. An elaborate self-consistency procedure is designed with the following salient features: (i) The Hamiltonian is rendered diagonal in a subspace of states of both an even and a neighboring odd nucleus. (ii) The Pauli principle, as represented by sum rules imposed on the coefficients of fractional parentage, is satisfied as accurately as possible in a least-squares sense. (iii) The number of particles is conserved exactly in all states of the system. Results of calculation for a simple model are compared with exact solutions and found to be vastly improved over previous results. The exact results were obtained by means of a new self-consistent version of exact shell-model diagonalization, which is described.

I. INTRODUCTION

IN the two previous papers[1–3] of this sequence, we developed methods of studying the ground and low-lying states of medium and heavy nuclei within the context of the pairing interaction Hamiltonian. These methods were based on the study of exact equations of motion for matrix elements of single-fermion operators (coefficients of fractional parentage, hereafter CFP), sum rules obeyed by the latter, and attendant self-consistency conditions. Approximations were devised which gave answers considerably improved over the BCS ones. Encouraged by these results, we here propose a more elaborate approximation scheme which, in fact, constitutes a self-consistent theory fully consonant with the inherent structure of the equations under study, and correcting all the shortcomings of our previous work, as we shall demonstrate. The main burden of the paper is to show how to improve systematically the computation of the properties of the low-lying states. It is also shown that a variant of our basic approach can be used to obtain exact solutions to the problem, and indeed was so utilized in the numerical examples considered.

What we have learned from previous experiences is that the equations-of-motion method, combined with spectral decomposition techniques, allows us to clarify and control, at each stage of development of the theory, the various approximations involved. This is of great value because we know at each level of complexity the next steps to be taken in order to move ever closer to the exact solution.

In the first paper (I) of this series, our interest was confined to ground states of even nuclei and to the one-quasiparticle states of the neighboring odd-mass nucleus. The aim was to correct the number nonconservation implicit in the BCS theory. This problem was reduced to that of calculating the differences of occupation numbers between two neighboring even nuclei,

$$\delta_\alpha = \langle 0(A)|\rho_\alpha|0(A)\rangle - \langle 0(A-2)|\rho_\alpha|0(A-2)\rangle, \quad (1.1)$$

where, in terms of the creation and annihilation operators of the shell model, $a_\alpha^\dagger$, a_α, $\rho_\alpha = a_\alpha^\dagger a_\alpha$. It turns out that the correction from this source constitutes the major step, insofar as the ground-state energy is concerned, in advancing from the BCS to the exact result.

The next step obviously required the introduction of excited states. Starting from the results of I for the ground state, this was done in II by using a version of the random-phase approximation (RPA). We thus defined the so-called one- (and two-) phonon states and matrix elements of the two-nucleon-transfer (gap) operators connecting these to the ground state. The crucial point was the assumption that these off-diagonal matrix elements were of first order of smallness. Subsequently all physical observables were calculated up to second order in these quantities. Concerning the ground-state energies, it was seen in II that inclusion of the contributions from these excited states gave us practically

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[1] G. Do Dang and A. Klein, Phys. Rev. **143**, 735 (1966), hereafter referred to as I.

[2] G. Do Dang and A. Klein, Phys. Rev. **147**, 689 (1966), hereafter referred to as II. I and II should be consulted for references to other approaches to the pairing problem.

[3] A few representative references on the pairing problem that have come to our attention since our previous work was published, from which the reader may trace competing and parallel developments, include K. Hara, Nucl. Phys. **A95**, 385 (1967); R. W. Richardson, Phys. Rev. **159**, 792 (1967); A. Covello and E. Salusti, *ibid.* **162**, 859 (1967); M. Jean, X. Campi, and H. Vucetick, in *Fundamentals in Nuclear Theory* (International Atomic Energy Agency, Vienna, 1967), p. 807; J. N. Ginochio and J. Weneser, Phys. Rev. **170**, 859 (1968).

the exact result. The excitation energies, however, were not well reproduced and errors of as much as 20% could be seen.

In the next section, we shall review this approximation and make a critical analysis of the assumptions which are supposed to be responsible for the observed discrepancies. In Sec. III we include a discussion of the utilization of the method of spectral decomposition. Section IV is reserved for a full account of the self-consistent theory and methods of solution. The novel method used to obtain exact solutions is exposed in Sec. V. Finally, results and discussion of the various approximations are given in Sec. VI. In all numerical examples illustrating the theory of this paper, we refer to a simple model with two levels of equal fourfold pair degeneracy ($\Omega_a=4$) with energies $h_a=0$ and 2 MeV. The pairing force strength is taken to be $G=0.50$ MeV and the numbers of particles of the three coupled systems to be studied are 4, 5, and 6.

The work described in this paper should be viewed as the spearhead of the necessarily more elaborate effort to treat spherical nuclei (as described by the pairing plus quadrupole interaction Hamiltonian) by similar methods, a program that is well under way.[4-6]

II. LINEARIZED APPROXIMATION

We shall adopt most of the notations of II. The seniority-zero states of an even-even nucleus with A active particles will be denoted by $|I(A)\rangle$ and the seniority-one states of the neighboring odd-mass nucleus by $|\alpha\nu(A-1)\rangle$, where α includes the angular momentum of the state. The relations between these systems are given by the following one-particle amplitudes (CFP):

$$\begin{aligned}\langle\bar{\alpha}\nu(A-1)|\,a_{\bar{\alpha}}^{\dagger}\,|I(A-2)\rangle&=u_{a\nu}(I,\,A-2)\,,\\ \langle\bar{\alpha}\nu(A-1)|\,s_\alpha a_\alpha\,|K(A)\rangle&=v_{a\nu}(K,A)\,,\end{aligned}\tag{2.1}$$

with $s_\alpha=(-)^{j_\alpha-m_\alpha}$.

From the pairing Hamiltonian

$$H=\sum_\alpha h_a a_\alpha^{\dagger}a_\alpha-\tfrac{1}{4}G(\sum_\alpha s_\alpha a_\alpha^{\dagger}a_{\bar{\alpha}}^{\dagger})(\sum_\beta s_\beta a_{\bar{\beta}}a_\beta)\,,\tag{2.2}$$

using the operator equations of motion, we obtain the following exact system of equations of motion for the CFP:

$$[E_{a\nu}-\epsilon_a-\omega_I(A-2)]u_{a\nu}(I,\,A-2)=\sum_K\Delta(KI)v_{a\nu}(K,A)\,,\tag{2.3}$$

$$[E_{a\nu}+\epsilon_a-\omega_K(A)]v_{a\nu}(K,A)=\sum_I\Delta(KI)u_{a\nu}(I,\,A-2)\,.\tag{2.4}$$

We recall the definition of the various quantities involved:

$$E_{a\nu}=W_{a\nu}(A-1)-\tfrac{1}{2}[W_0(A)+W_0(A-2)]+\tfrac{1}{2}G\,,\tag{2.5}$$

$$\omega_I(A)=W_I(A)-W_0(A)\,,\tag{2.6}$$

$$\lambda(I)=\tfrac{1}{2}[W_I(A)-W_I(A-2)]\,,\tag{2.7}$$

$$\lambda_1=\lambda(0)+\tfrac{1}{2}G,\quad \epsilon_a=h_a-\lambda_1\,,\tag{2.8}$$

$$\Delta(KI)=\tfrac{1}{2}G\sum_\alpha\langle I(A-2)|\,s_\alpha a_{\bar{\alpha}}a_\alpha\,|K(A)\rangle=G\sum_{a\nu}\Omega_a u_{a\nu}(I,\,A-2)v_{a\nu}(K,A)\,.\tag{2.9}$$

The only difference compared with the notations of II is the definition of the "chemical potentials" $\lambda(I)$, not only for the ground states, but also for excited states. Though $\lambda(I)$, $I\neq0$, does not occur in (2.3) and (2.4) as written, it is clear that it will occur as soon as we decide to refer excitation energies to a definite one of the two neighboring even nuclei.

Equations (2.3) and (2.4) are to be viewed as an eigenvalue equation for $E_{a\nu}$ if the various quantities (2.6)–(2.9) are known. A viable approximation scheme must specify a systematic or iterative scheme for improving our knowledge of these quantities.

At any given stage of the full calculational scheme, our momentary knowledge of (2.5)–(2.9) (knowledge of the core properties and of the core-particle interaction) enables us to find a set of vectors with components $u_{a\nu}(I,\,A-2)$, and $v_{a\nu}(K,A)$ which characterize the states of the odd nucleus. These vectors are normalized by using the Pauli principle and the number conservation which are written in the form

$$\sum_{a\nu}\{v_{a\nu}(K,A)v_{a\nu}(K',A)+u_{a\nu}(K,A)u_{a\nu}(K',A)\}=\delta_{KK'}\,,\tag{2.10}$$

$$\sum_{a\nu}2\Omega_a v_{a\nu}(K,A)v_{a\nu}(K',A)=A\,\delta_{KK'}\,,\tag{2.11}$$

and similarly for the system $A-2$. Note that in Eq. (2.10), only one system is involved while in Eqs. (2.3) and (2.4) the amplitudes for both systems (A) and $(A-2)$ intervene. This is the main point emphasized in I and also, as we shall see, is of crucial importance for what follows.

As a matter of fact, all excited states are neglected in I so that the system (2.3)–(2.4) is there reduced to the usual BCS equations. The improvement comes from the realization that the quantity δ_a defined in (1.1) may differ appreciably from the BCS value (zero) so that we get, from Eq. (2.10), the normalization condition

$$u_a^2(A-2)+v_a^2(A)=1+\delta_a\,,\tag{2.12}$$

using standard notation. In I, we gave two ways to calculate δ_a, which then completely defines the ground state.

[4] G. Do Dang and A. Klein, Phys. Rev. **156**, 1159 (1967).
[5] R. M. Dreizler, A. Klein, Chi-Shiang Wu, and G. Do Dang, Phys. Rev. **156**, 1167 (1967).
[6] G. Do Dang, R. M. Dreizler, A. Klein, and Chi-Shiang Wu, J. Phys. Soc. Japan, Suppl. **24**, 568 (1968).

To go one step further, one must introduce excited states. This was done in II by using a linearization procedure well known from the random-phase approximation (RPA), and owing to the fact that we conserve particles exactly in the ground state, we shall term it loosely the number conserving RPA. Instead of rewriting some of the results obtained in II, we shall recall the basic ideas contained in this approximation. The fundamental assumption is that there are excited states such that the matrix elements of the gap operator, Eq. (2.9), between them and the ground states are small and can be taken to be of first order. The linearization of the equations of motion for these matrix elements leads immediately to a dispersion equation defining the excitation energies. Systematic use of normalization conditions and the Pauli principle, as an adjunct to the equations of motion, defines these matrix elements completely (we simply call these RPA amplitudes henceforth) and permits us to calculate all observables up to second order in these quantities. We recall, for example, that the excitation energies ω_I can be expressed as a sum over terms all of second order [see II, Eq. (4.8)].

Besides the above assumption, others that are needed to put the solution into closed form, will now be analyzed.

(A) The number conservation is relaxed. The failure to conserve the number of particles exactly manifests itself in three different ways:

(1) As is well known, in the RPA, the definition of the phonon states presupposes the knowledge of the ground state. As a consequence, all the parameters related to the ground state are left unchanged, in particular, the chemical potential. Fixing this quantity in advance reduces the freedom to conserve the number of particles in the ground state, since this number is modified by the presence of the excited states.

(2) A similar assumption is to take $\omega_I(A)=\omega_I(A-2)$. But, in terms of the chemical potentials $\lambda(I)$ for excited states, the difference

$$\tfrac{1}{2}[\omega_I(A)-\omega_I(A-2)]=\lambda(I)-\lambda(0) \qquad (2.13)$$

should be used to fix the number of particles in the corresponding excited state.

(3) The third number nonconserving approximation which has been made is based on the assumed smallness of the RPA amplitudes. As a result, no care has been taken to distinguish the values in the two systems A and $A-2$.

As it turns out, numerical examples show that assumptions (1) and (3) are more or less satisfied, while assumption (2) may not be and sometimes leads to errors of up to 10% in the number of particles in the excited states.

(B) The self-consistency problem is simply neglected. By this we mean the following: In the definition of the one-phonon state, as mentioned above, all the properties of the ground state are kept unchanged. More seriously, some of them are assumed to be the same in the ground state and in excited states. For example, use has been made of the approximate equalities $\Delta(II)\cong\Delta(00)\cong\Delta^{(0)}$ and also the particle occupation numbers are supposed unchanged. But, once the phonon states are completely defined, all these quantities can be recalculated up to second order in the RPA amplitudes. The neglect of self-consistency then simply means that no effort has been made to redefine the phonon states, using these newly calculated parameters. As the latter may differ appreciably from the original ones, this neglect may be serious. For example, we have found that $\Delta(II)$ may be smaller than $\Delta^{(0)}$ by as much as 30% (blocking effect), and that the excitation energies calculated from them are greatly affected. This is so because roughly

$$\omega_I\sim(4\Delta^2+\chi^2), \qquad (2.14)$$

where χ is defined by a phonon dispersion equation [Eq. (3.22) in II] and depending on whether we use $\Delta(II)$ or $\Delta^{(0)}$ for Δ in (2.14), the values obtained for ω_I may differ appreciably from each other. It has been found that, in the approximation of Paper II, the values of ω_I are usually overestimated.

Before we go further to correct these deficiencies and in order to get an idea of the role played by the intermediate states in the decomposition process, the following discussion will hopefully clarify these matters and lead us closer to the self-consistent theory.

III. INTERMEDIATE STATES IN SPECTRAL DECOMPOSITION

It is well known from the RPA that the so-called two-phonon states are assumed to exist if the one-phonon states do. They are defined as the direct products of two one-phonon states, of the form

$$|I+I'\rangle=(|I\rangle\otimes|I'\rangle)(1+\delta_{II'})^{-1/2}. \qquad (3.1)$$

This form has the special property that all matrix elements connecting these states to the one-phonon states can be reduced; for example,

$$\Delta(I+I', I)=(1+\delta_{II'})^{1/2}\Delta(I'0). \qquad (3.2)$$

As a consequence, and though the two-phonon states seem to be present nowhere in the equations of motion for the one-phonon states, they do play a role as intermediate states in the decomposition process. For example, suppose we have to calculate the matrix elements of the product AB of two operators between two one-phonon states $I\neq I'$. We obtain from (3.2), keeping only terms of second order,

$$\begin{aligned}\langle I|AB|I'\rangle=&\{\langle I|A|0\rangle\langle 0|B|I'\rangle\}\\&+\{\langle I|A|I\rangle\langle I|B|I'\rangle+\langle I|A|I'\rangle\langle I'|B|I'\rangle\}\\&+\{\langle 0|A|I'\rangle\langle I|B|0\rangle\}, \qquad (3.3)\end{aligned}$$

where the various braces contain the contributions from the zero-, one-, and two-phonon intermediate states.

How large the contributions from two-phonon states actually are depends on the problem at hand, and more specifically, on the size of the matrix elements connecting them to the one-phonon states. The only simple alternative to treating their contribution to (3.3) as dictated by (3.1) and (3.2) is to leave them out altogether. Both alternatives can only be checked by a better calculation.

In the self-consistent theory described in the next section, our aim is to avoid *a priori* physical prejudices such as contained in the phonon picture and expressed by Eq. (3.2). We retain some aspects of this picture only in the continued assumption of classes of preferred intermediate states. We calculate the properties of a number of states simultaneously, but this does not imply, by any means, that these properties are given with equal accuracy for all the states. Only those states are accurately represented whose properties are insensitive to the enlargement of the problem. In some cases it is not difficult to decide on physical grounds which states may be so considered, without making additional calculations. As an example of this, we know that with the inclusion of the so-called one-phonon states we have obtained most of the important corrections to the ground-state properties.

IV. SELF-CONSISTENT THEORY

Let us make a preliminary remark about the system of equations (2.3) and (2.4). As written, the summation over states of the even-even nuclei includes as many states as we wish and it is not necessary that the numbers of states in the systems A and $A-2$ be equal. We shall suppose, however, that, as far as the lowest-lying states are concerned, the ones in which we are most interested, we can definitely make a close correspondence between the states of the two systems. In the RPA, this is effectively the case: We have as many one- (and two-) phonon states in system A as in system $A-2$. We should always remember, however, never to assign to any system more states than it can possess. In the example of this paper, the system $A=6$ has 4 seniority-zero states while system $A=4$ has only 3. In this case, it does not make sense to talk about three-phonon states.

We now turn to the self-consistency technique, which replaces the linearization procedure formerly used. As the discussion which follows is rather elaborate we summarize beforehand its salient elements:

(i) We solve Eqs. (2.3) and (2.4) for the $E_{a\nu}$, $v_{a\nu}$, $u_{a\nu}$ assuming that we know the ω, ϵ, Δ that define the "Hamiltonian."

(ii) A subset of solutions of (2.3) and (2.4), identified as "physical", is retained and normalized by means of the Pauli principle (2.10) or (4.2) below. This implies a knowledge of the quantities $\delta_a(I,I')$ of (4.3).

(iii) With the normalized solutions thus obtained, the energy matrix (4.9) of the core system is formed and diagonalized. The transformation matrix that accomplishes this yields an improved set of vectors $v_{a\nu}$ and $u_{a\nu}$, according to (4.10). From the point of view of principle, the $\lambda(I)$ and $\lambda(0)$ are now adjusted to conserve the number of particles in each state $|I(A)\rangle$. Altogether these steps yield a new set of ω, ϵ, Δ with which the entire procedure may be repeated until over-all self-consistency is reached.

(iv) All of the above is for a fixed $\delta_a(I,I')$, Eq. (4.3). A self-consistent method for obtaining the correct value of the latter is described, which requires additional repetition of steps (i)–(iii).

(v) From the results, all physical quantities relating to all states included in the calculation can be obtained.

As has been said above, the system (2.3)–(2.4) is an eigenvalue equation for $E_{a\nu}$. The first problem is to define the quantities ω, ϵ, Δ in a self-consistent way. For definiteness, we shall suppose that we start from the RPA solution. Let p be the number of states of an even system which are considered. The diagonalization of the secular matrix gives at the same time $2p$ eigenvalues $E_{a\nu}$ and $2p$ eigenvectors $\psi_{a\nu}{}^{(0)}$ with components $u_{a\nu}{}^{(0)} \times(I, A-2)$ and $v_{a\nu}{}^{(0)}(I,A)$, $(I=1\cdots p)$. These vectors satisfy orthogonality relations following from (2.3) and (2.4), which, together with an *arbitrary* assumption about normalization, may be expressed as

$$\sum_I \{u_{a\nu}{}^{(0)}(I, A-2)u_{a\nu'}{}^{(0)}(I, A-2) + v_{a\nu}{}^{(0)}(I,A)v_{a\nu'}{}^{(0)}(I,A)\} = \delta_{\nu\nu'}. \quad (4.1)$$

There are at this point two problems requiring immediate resolution.

(i) As in the simple BCS case there is a doubling of solutions. We have to select from the $2p$ solutions, p physical ones. These can be identified unambiguously in the limit in which the pairing matrix $\Delta(KI)$ of Eq. (2.9) is diagonal. We then ask if it is possible to follow the solutions from this limit in a continuous way. We give in the Appendix all the details of a method to achieve this end.

(ii) The vectors obtained from the diagonalization are not properly normalized. Each physical state vector $\psi_{a\nu}{}^{(0)}$ has to be multiplied by a factor $\mu_{a\nu}$ such that the Pauli principle (2.10) is satisfied. To do this, we rewrite (2.10) in the form

$$\sum_\nu \{u_{a\nu}(I, A-2)u_{a\nu}(I', A-2)+v_{a\nu}(I,A)v_{a\nu}(I',A)\} = \delta_{II'}+\delta_a(I,I'), \quad (4.2)$$

where by definition

$$\delta_a(I,I') = \langle I(A)|\rho_\alpha|I'(A)\rangle - \langle I(A-2)|\rho_\alpha|I'(A-2)\rangle, \quad (4.3)$$

which are the analogs of δ_a in (1.1) and are to be defined by some sequential method of calculation. In the BCS theory, all $\delta_a(I,I')$ are taken to be zero. Suppose for a moment that these quantities are known in some approximation; the calculation problem of normalization

constants is then well defined. We have in fact in Eq. (4.2) a system of $p'=p(p+1)/2$ equations from which p solutions $\mu_{a\nu}{}^2$ (for each a) are to be determined. We shall therefore determine a set of solutions $\mu_{a\nu}{}^2$ which, in a least-squares sense, satisfy best the whole system of equations (4.2). This is done as follows. The system (4.2) can be written as

$$AX=B, \tag{4.4}$$

where X is the vector with components $(\mu_{a1}{}^2, \mu_{a2}{}^2, \cdots, \mu_{ap}{}^2)$, and A is a p'-by-p rectangular matrix. The vector X is now determined by the requirement that any infinitesimal variation of X from the best solution will leave invariant the quadratic form

$$Q=\sum_i [\sum_j A_{ij}X_j-B_i]^2. \tag{4.5}$$

We obtain the p equations

$$\partial Q/\partial X_k=0=\sum_i(\sum_j A_{ij}X_j-B_i)A_{ik} \tag{4.6}$$

or

$$A'X=B', \tag{4.7}$$

where

$$\begin{aligned} A_{ij}{}'&=\sum_k A_{ki}A_{kj}, \\ B_i{}'&=\sum_k A_{ki}B_k; \end{aligned} \tag{4.8}$$

Eqs. (4.7) can now be solved for X. It is important to remark that the renormalization of the physical state vectors does not destroy the orthogonality among these vectors.

We next require that the Hamiltonian be diagonal in the subspace of the p states of the even system. This is because the form of Eqs. (2.3) and (2.4) is based on that assumption, which must now be verified *a posteriori*. The solutions $\psi_{a\nu}$ just found permit us to calculate the matrix of this Hamiltonian in the form

$$\begin{aligned} \langle I(A)|H|I'(A)\rangle=&\sum_{a\nu} 2\Omega_a h_a v_{a\nu}(I,A)v_{a\nu}(I',A) \\ &-G\sum_{I''}[\sum_{a\nu}\Omega_a u_{a\nu}(I'',A-2)v_{a\nu}(I,A)] \\ &\times[\sum_{b\nu'}\Omega_b u_{a\nu'}(I'',A-2)v_{a\nu'}(I',A)]. \end{aligned} \tag{4.9}$$

In the present method the summation I'' includes all (and only) the states considered in the problem. The diagonalization of (4.9) defines a transformation T on the basis of the even system A, and thus a new set of one-particle amplitudes $v_{a\nu}{}'(I,A)$:

$$v_{a\nu}{}'(I,A)=\sum_{I'}[T(I,I')v_{a\nu}(I',A)], \tag{4.10}$$

where we suppose that this transformation defines at the same time a change of basis in the system $A-2$. It is at this point that the assumption that there exists a correspondence between states of the two systems manifests its full meaning. We could also think of defining a separate transformation for system $A-2$ by a diagonalization of the Hamiltonian matrix for this system. The latter can, by algebraic manipulation, be put into a form such that the solutions $\psi_{a\nu}$, already found, suffice for this calculation. But, the justification for this procedure requires the Pauli principle to be satisfied between states of different seniorities, a condition that we have nowhere imposed.

The diagonalization of (4.9) not only defines a basis transformation but also the total energies of the system, namely, $W_I(A)$, the eigenvalues. We are, consequently, in a position to define a new set of input parameters. First, we get

$$\omega_I{}'(A)=W_I(A)-W_0(A). \tag{4.11}$$

The matrix elements $\Delta'(II')$ of the gap operator can also be calculated from (2.9). These are generally different from the values we use as input. In principle, we iterate the entire procedure for a fixed set of values of $\delta_a(I,I')$, Eq. (4.3), until self-consistency is achieved. This means that (4.9) is diagonal and all parameters needed in (2.3) and (2.4) have settled down to fixed values. To achieve this in practice, we have followed the procedure of calculations which we now outline:

(i) As we start from the parameters obtained from the RPA, we first keep constant the RPA amplitudes $\Delta(I0)$ [and eventually $\Delta(I+I', I)$ when two-phonon states are present]. We then can choose a set of values $\omega_I(A)$, and consequently $\omega_I(A-2)=\omega_I(A)+2(\lambda(I)-\lambda(0))$ [for use in the equations of motion] such that these amplitudes are identical with the corresponding ones calculated from (2.9). At each step of the iteration, the values of other matrix elements $\Delta(II')$ are taken from the previous cycle. The method for obtaining $\lambda(I)$ will be described below.

(ii) We then renormalize the RPA amplitudes so that $\omega_I{}'=\omega_I$. A criterion for doing this can be obtained from the remark that, in the RPA, $\omega_I \propto \Delta^2(I0)$. Technically, there are many satisfactory ways in which these steps can be incorporated into the program.

Once these two steps have been carried out, we have at our disposal a set of one-particle amplitudes which define at the same time a basis of the even systems $|I(A)\rangle$ and that of the odd mass system $|\alpha\nu\rangle$ such that the Hamiltonian is diagonal. At this juncture the number of particles in the states of the even systems has not yet been properly specified; we shall use this fact to determine the remaining parameters in the secular matrix, resulting from (2.3) and (2.4). We impose the condition that the diagonal matrix elements of the number operator in the system A, as given by (2.11), be equal to A. Each parameter $\lambda(I)$ then will be used to satisfy this requirement for the state $|I\rangle$. Remark that no condition is imposed on the off-diagonal matrix elements: These will be used as a check of the ultimate consistency of the theory. An alternative here would be another least-squares fitting procedure.

There remain finally the quantities $\delta_a(I,I')$ to be determined. This is done by extending a method given in I in the following way: Instead of imposing the conservation of the number of particles for system A, we could equally well conserve the numbers of holes in system $A-2$ which are given by

$$N_h(A-2)=\sum_{a\nu} 2\Omega_a u_{a\nu}(I,\,A-2)u_{a\nu}(I,\,A-2). \quad (4.12)$$

Depending on whether we use (2.11) or (4.12), we obtain at convergence different sets of parameters. From the first set, with the use of (2.11), we find the values of

$$n_a(I,I',A)=\langle I(A)\,|\,\rho_\alpha\,|\,I'(A)\rangle. \quad (4.13)$$

From the second set, we find

$$n_a(I,\,I',\,A-2)=\delta_{I,I'} -\langle I(A-2)\,|\,a_\alpha a_\alpha{}^\dagger\,|\,I'(A-2)\rangle. \quad (4.14)$$

Starting with the BCS values $\delta_a{}^{(0)}(I,I')=0$, we now generate a new set:

$$\delta_a{}^{(1)}(I,I')=n_a(I,I',A)-n_a(I,\,I',\,A-2). \quad (4.15)$$

The entire process of iteration can now be repeated with these new parameters, and so on until convergence, which is reached when

$$\delta_a{}^{(n+1)}(I,I')=\delta_a{}^{(n)}(I,I'). \quad (4.16)$$

At this point, using (2.11) or (4.12) gives the same set of parameters for the whole problem.

A remark should be made about the convergence of the iteration. We have found that the parameters connected with excited states are often far different from those connected with the ground state. Starting with parameters of the RPA, special care has to be taken at the start of the iteration process in order to assure that the final solutions are those sought. Details of a technique to assure the convergence are given in the Appendix.

V. METHOD FOR EXACT SOLUTION

In simple models, as the one employed in the numerical calculations in this paper, where the total number of states of the system is not too large, one can push the theory given above far enough, i.e., take into account states of higher energies, to get nearly exact results. If the number of states is too large, however, there may be difficulties in obtaining convergence in a finite computing time because the final results may differ too much from the ones we are able to guess as input values. We shall show in this section that, with appropriate modifications, the equations of motion lead us to an exact method of solution. In the course of our considerations, we shall derive a new sum rule for the pairing theory.

First, we remark that, up to now we have been working with matrix elements relating states of even systems among themselves or with states of the neighboring odd system. To get matrix elements of one-particle operators between states of the odd mass system requires the knowledge of the wave functions of these states. This can be done as follows: From the form of the equations of motion (2.3) and (2.4), we can write the wave function of a state $|\alpha\nu(A-1)\rangle$ in the form

$$|a\nu(A-1)\rangle=\lambda_{a\nu}\{\sum_I u_{a\nu}(I,\,A-2)a_\alpha{}^\dagger\,|\,I(A-2)\rangle -\sum_K v_{a\nu}(K,A)s_\alpha a_{\bar\alpha}\,|\,K(A)\rangle\}. \quad (5.1)$$

These states are orthonormalized, so that we have

$$\lambda_{a\nu}\{\sum_I u_{a\nu}(I,\,A-2)u_{a\nu'}(I,\,A-2) +\sum_K v_{a\nu}(K,A)v_{a\nu'}(K,A)\}=\delta_{\nu\nu'}. \quad (5.2)$$

Note that in this exact case, the sum of $K(A)$ may be different from the sum over $I(A-2)$.

In the approximate self-consistent theory of the previous section, as $u_{a\nu}(I,\,A-2)$ and $v_{a\nu}(I,A)$ are proportional to $u_{a\nu}{}^{(0)}(I,\,A-2)$ and $v_{a\nu}{}^{(0)}(I,A)$, respectively, we see from Eq. (4.1) that the choice

$$\lambda_{a\nu}=1/\mu_{a\nu}{}^2, \quad (5.3)$$

where $\mu_{a\nu}$ is defined by (4.2), will satisfy Eq. (5.2).

In the case of an exact calculation where the sums on I and K run over all existing seniority-zero states, we can write the wave functions of the states of the odd mass systems, not only in the form (5.1), but also in the following ways:

$$|\alpha\nu\rangle=\sum_I A_{a\nu}(I)a_\alpha{}^\dagger\,|\,I(A-2)\rangle, \quad (5.4)$$

$$|\alpha\nu\rangle=-\sum_K B_{a\nu}(K)s_\alpha a_{\bar\alpha}\,|\,K(A)\rangle. \quad (5.5)$$

This is so because the basis defined by the different terms in the sums is, in each case, at least sufficient to characterize all the seniority-one states of the system $A-1$. $A_{a\nu}(I)$ and $B_{a\nu}(K)$ are coefficients that can be determined if required.

We now show that the coefficients $\lambda_{a\nu}$ can be calculated exactly and are given by

$$\lambda_{a\nu}=\Omega_a/(1+\Omega_a), \quad (5.6)$$

which are independent of ν. To show this, we use the Pauli principle, which we now write in the form

$$(1/2\Omega_a)\langle\alpha\nu\,|\sum_{m_{\alpha'}}(a_{\alpha'}{}^\dagger a_{\alpha'}+a_{\alpha'}a_{\alpha'}{}^\dagger)\,|\,\alpha\nu'\rangle=\delta_{\nu\nu'}, \quad (5.7)$$

where $a'=a$. Using (5.5), we get for the first sum in (5.7)

$$\begin{aligned}\langle\alpha\nu\,|\sum_{m_{\alpha'}}a_{\alpha'}{}^\dagger a_{\alpha'}\,|\,\alpha\nu\rangle&=-\sum_{K,m_{\alpha'}}B_{a\nu'}(K)\\ &\times\langle\alpha\nu\,|\,a_{\alpha'}{}^\dagger a_{\alpha'}s_\alpha a_{\bar\alpha}\,|\,K(A)\rangle\\ &=\sum_K B_{a\nu'}(K)\langle a\nu\,|\,s_\alpha a_{\bar\alpha}\,|\,K(A)\rangle\\ &\quad-\sum_{K,m_{\alpha'}}B_{a\nu'}(K)\langle\alpha\nu\,|\,a_{\bar\alpha}a_{\alpha'}{}^\dagger a_{\alpha'}\,|\,K(A)\rangle\\ &=-\sum_K B_{a\nu'}(K)v_{a\nu}(K,A)+2\Omega_a\sum_{K,\nu''}v_{a\nu}(K,A)v_{a\nu''}(K,A)\\ &\quad\times\sum_{K'}B_{a\nu'}(K')v_{a\nu''}(K',A). \end{aligned} \quad (5.8)$$

But the states (5.5) are orthonormal by definition; namely,

$$\sum_K B_{a\nu}(K)v_{a\nu'}(K,A)=\delta_{\nu\nu'}, \tag{5.9}$$

so that (5.8) yields

$$\langle\alpha\nu|\sum_{m_{\alpha'}} a_{\alpha'}{}^{\dagger}a_{\alpha'}|\alpha\nu'\rangle=-\delta_{\nu\nu'} +2\Omega_a\sum_K v_{a\nu}(K,A)v_{a\nu'}(K,A). \tag{5.10}$$

The same thing can be done for the second sum in (5.7), using (5.4) and we arrive at the final result:

$$\sum_I u_{a\nu}(I,A-2)u_{a\nu'}(I,A-2)+\sum_K v_{a\nu}(K,A)v_{a\nu'}(K,A) =[1+(1/\Omega_a)]\delta_{\nu\nu'}. \tag{5.11}$$

Comparing this sum rule with the orthogonality relations (5.2), we obtain Eq. (5.6). This result (5.6) shows at least one thing: The vectors obtained from the diagonalization of the secular matrix (2.3) and (2.4) are, except for the trivial BCS case, not of unit norm. We have discussed this matter elsewhere in somewhat greater generality,[7] pointing out the shortcomings in the existing literature in this respect.

Using the above result and various physical requirements, we now show how exact solutions can be obtained. Suppose we know a set of one-particle amplitudes $u_{a\nu}{}^{(0)}(I,A-2)$ and $v_{a\nu}{}^{(0)}(K,A)$, which, as a matter of fact, can be chosen almost arbitrarily. The exact solution is then obtained by iterating the following three steps, in the order indicated.

(1) We first require that the number operator be diagonal in the basis of states $|K(A)\rangle$ with diagonal elements all equal to A. Starting from the basis $|K(A)\rangle_{(0)}$ defined by $u^{(0)}$ and $v^{(0)}$, we make a transformation

$$|K(A)\rangle_{(1)}=\sum_{K'} C_{KK'}{}^{(1)}|K'(A)\rangle_{(0)}, \tag{5.12}$$

such that

$${}_{(1)}\langle K(A)|N|K'(A)\rangle_{(1)}=A\delta_{KK'}. \tag{5.13}$$

The problem is then equivalent to the diagonalization of the matrix

$${}_{(0)}\langle K(A)|N|K'(A)\rangle_{(0)} =\sum_{a\nu} 2\Omega_a v_{a\nu}{}^{(0)}(K,A)v_{a\nu}{}^{(0)}(K,A), \tag{5.14}$$

followed by the renormalization of the eigenvectors according to (5.13). We thus define the matrix $C^{(1)}$ and consequently a new set of one particle amplitudes $v_{a\nu}{}^{(1)}\times(K,A)$ in a way similar to the transformation (4.10). An analogous procedure is then applied to system $A-2$ by normalizing the number of holes and thus defining a new set $u_{a\nu}{}^{(1)}(I,A-2)$. The two problems can be done without any difficulty if in the two cases the input $u^{(0)}$, $v^{(0)}$ is such that the diagonalizations never lead to a vanishing eigenvalue. This is the first condition imposed on the input.

(2) The second step consists in the definition of two more transformations which diagonalize the Hamiltonian. This is done as above, but now these transformations are orthogonal because no renormalization of eigenvalues is involved. As a consequence of this fact, in the new basis, $|K(A)\rangle_{(2)}$ and $|I(A-2)\rangle_{(2)}$, the number operators are still diagonal. We thus define a new set of amplitudes $u_{a\nu}{}^{(2)}(I,A-2)$ and $v_{a\nu}{}^{(2)}(K,A)$.

(3) In this final step, we require the Hamiltonian to be diagonal in the basis defined by (5.1) and (5.6). Here, there is a little problem, however, which arises from the fact that with the set of input parameters obtained from the previous step, there is no reason to expect this basis to be orthonormal. Let us define the following matrices (the index a is omitted):

$$M_{\nu\nu'}=\langle\alpha\nu|\alpha\nu'\rangle, \tag{5.15}$$

$$D_{\nu\nu'}=\langle\alpha\nu|H|\alpha\nu'\rangle, \tag{5.16}$$

which can be expressed in terms of the $u_{a\nu}{}^{(2)}(I,A-2)$ and $v_{a\nu}{}^{(2)}(K,A)$, using (5.1) and commutation relations. Let S be the matrix of basis transformation. It is easy to show that it is formed from the set of eigenvectors V of the following eigenvalue equation, well known in the theory of small vibrations:

$$WMV=DV, \tag{5.17}$$

where the eigenvalues are the total energies of the odd mass system. The problem can be reduced to the usual form by defining a matrix T such that

$$TMT^{-1}=I, \tag{5.18}$$

with I being the identity matrix. We then have from (5.17)

$$WV'=D'V', \tag{5.19}$$

with $V'=TV$, $D'=TDT^{-1}$. The diagonalization of D' gives W and V' and consequently V. The matrix S constructed from V, which is used to define a new set of parameters $u_{a\nu}{}^{(3)}(I,A-2)$ and $v_{a\nu}{}^{(3)}(K,A)$, is normally not unitary because T is not an orthogonal transformation, at least in the first few steps of iteration. Note that T can be obtained only if the diagonalization of M does not lead to any nonvanishing eigenvalue. This is the second condition imposed on the initial input. In any event, we can now use $u^{(3)}$ and $v^{(3)}$ as new input and then repeat the three-step process until convergence. When this is reached, all transformations become identity transformations.

In simple models where we have available some set of single-particle CFP, from the shell model, the above procedure reduces to the standard shell-model problem,

[7] G. Do Dang, G. J. Dreiss, R. M. Dreizler, A. Klein, and Chi-Shiang Wu, Nucl. Phys. (to be published).

TABLE I. Comparison of the parameters defining the ground state in different approximations. Refer to the end of Sec. I for the values of input parameters. See Sec. II for a definition of all parameters.

	BCS	I	RPA	II	IIIa	IIIb	Exact
$W_0(6)$	−4.1037	−5.0216	−4.1712	−5.0654	−5.0850	−5.0709	−5.0724
$\lambda(0)$	0.0939	−0.2302	0.0939	−0.2302	−0.2708	−0.2684	−0.2683
$\Delta(00)$	1.6952	1.9280	1.6340	1.8930	1.8874	1.8866	1.8870
$\Delta(11)$			1.3041	1.6024	1.4050	1.3644	1.3618
$\Delta(22)$						0.9558	0.9358

requiring but a single diagonalization in each space of A, $A-2$, and $A-1$ particles, i.e., a single cycle of three steps.

VI. RESULTS AND DISCUSSION

In the two-level model considered as example in this paper, the RPA defines a single one-phonon state and one two-phonon state. We have solved this problem in various approximations with the results given in Tables I–V. The approximations considered are as follows:

(1) The usual BCS approximation (denoted by BCS).
(2) The usual RPA (RPA).
(3) The number-conserving approximation of I.
(4) The number-conserving RPA of II.
(5) The self-consistent theory of Sec. IV with (a) the even systems defined by two states, the ground state and the one-phonon state (column IIIa) of the tables, (b) the even systems defined by three states, the ground state and the one- and two-phonon states (column IIIb of the tables).
(6) The exact solution (Exact).

TABLE II. Comparison between the RPA amplitudes obtained in various approximations. All quantities in parentheses in this and succeeding tables are not explicitly calculated, but follow instead from the assumption of a pure phonon spectrum.

	RPA	II	IIIa	IIIb	Exact
$\Delta(01)$	0.2046	0.1627	0.1022	0.0999	0.1001
$\Delta(10)$	0.5159	0.5080	0.5786	0.5829	0.5774
$\Delta(12)$	(0.2893)	(0.2300)		0.0421	0.0425
$\Delta(21)$	(0.7294)	(0.7183)		0.8032	0.8198

From the results obtained, the following remarks can be made concerning these approximations, identified as above:

(1) As is well known, the BCS approximation gives poor results for the ground-state energy. The wave function as represented by the occupation numbers, $\langle 0|\rho_a|0\rangle$, is fairly good. Note also that the gap is not well reproduced.

(2) The usual RPA, which is defined from the BCS ground state, contains the same deficiencies, as far as the ground state is concerned. The excitation energies, at least those connected with one-phonon states, are not well reproduced. They are underestimated.

(3) The simple number-conserving approximation definitely gives very good results for the ground-state energy, as has also been observed in I for other models. The occupation numbers, however, do not seem to change much.

(4) For the ground-state energy, the contributions from excited states practically fill up the gap between that given by (3) and the exact solution. The excitation energies, however, are usually overestimated. This can be understood from the remark following (2.15) and from the fact that while $\Delta(00)$ is well-reproduced, the use of this value for excited states is not justified.

In relation to the analysis of Sec. II B, we find that the number conservation is still good for the ground state. For excited states, however, it is badly violated. From Table III, for example, we have $\langle 1(A)|N|1(A)\rangle = 5.5$ instead of the correct value $A=6$.

(5) The self-consistent theory seems to improve results in all respects. It is gratifying first to remark that we were able to find the solution in a continuous way from that of the RPA. As a result and though the initial and final solutions may differ appreciably from each

TABLE III. The values of the occupation numbers of single-particle levels in various core states, $\langle I(A)|\rho_a|I(A)\rangle$, are given for various approximations.

a	I	BCS	I	RPA	II	IIIa	IIIb	Exact
1	0	0.5994	0.5992	0.6310	0.6269	0.6212	0.6210	0.6207
	1	(0.5994)	(0.5992)	0.6309	0.6166	0.5156	0.5304	0.5321
	2	(0.5994)	(0.5994)				0.3004	0.3073
2	0	0.1506	0.1508	0.1263	0.1340	0.1288	0.1291	0.1293
	1	(0.1506)	(0.1508)	0.0506	0.0705	0.2343	0.2197	0.2179
	2	(0.1506)	(0.1508)				0.4495	0.4427

TABLE IV. The values of the parameters $\delta_a(I,I)$ defined in Eq. (4.3).

a	I	I+II	IIIa	IIIb	Exact
1	0	0.1861	0.2016	0.1990	0.1991
	1	(0.1861)	0.2519	0.2355	0.2513
	2	(0.1861)		0.2563	0.2597
2	0	0.0639	0.0484	0.0509	0.0509
	1	(0.0639)	−0.0018	−0.0035	−0.0013
	2	(0.0639)		−0.0062	−0.0097

other, we still can talk about one- and two-phonon states. It is also worth remarking that the solution for the problem for system A gives at the same time that of system $A-2$. From Tables I and V we get, for example, $W_0{}^a(A-2)=-4.5435$, $\omega_1{}^a(A-2)=4.8781$ for the approximation (IIIa), and $W_0{}^b(A-2)=-4.5341$, $\omega_1{}^b\times(A-2)=5.0317$, $\omega_2{}^b(A-2)=10.6054$ for the approximation IIIb, which are to be compared with the exact solution $W_0{}^e(A-2)=-4.5358$, $\omega_1{}^e(A-2)=4.9693$ and $\omega_2(A-2)=10.6381$.

The number conservation can be enforced as accurately as desired for all states of the even systems by fixing the $\lambda(I)$. Though $\lambda(0)$ is almost the value given by II, $\lambda(I)$ for excited states are far from equal to $\lambda(0)$. This proves that the assumption $\omega_I(A)\sim\omega_I(A-2)$ cannot be trusted.

TABLE V. The excitation energies and the values of the chemical potentials for excited states in different approximations.

	RPA	II	IIIa	IIIb	Exact
ω_1	3.7593	4.4983	4.2163	4.1801	4.1801
ω_2	(7.5186)	(8.9966)		9.1448	9.0573
$\lambda(1)$	(0.0939)	(−0.2302)	−0.6017	−0.6942	−0.6629
$\lambda(2)$	(0.0939)	(−0.2302)		−0.9987	−1.0587

It is gratifying also to remark that though no effort has been made to diagonalize the number operators, all the off-diagonal elements remain negligible ($\sim10^{-3}$ compared to the diagonal value 6) throughout the iteration.

Further extensions of this work within the context of seniority-conserving interactions are planned: (i) numerical calculations for a larger number of single-particle levels; (ii) extending the method to interactions with nonconstant pairing matrix elements and monopole interactions; (iii) efforts to devise a method that remains completely within the subspace of even nuclei are also under way.

APPENDIX

In this Appendix, we shall give the details of a method of iteration that allows us to start from the RPA and get the self-consistent solution in a continuous way.

We recall that the RPA is based on the assumption that there exist the RPA amplitudes which are small; all physical observables are then developed up to second order in these amplitudes. Suppose then that in the secular equation (2.3) and (2.4) we multiply all the RPA amplitudes by a common small parameter η. The diagonalization of the secular matrix and the normalization of the eigenvectors obtained lead to the definition of new amplitudes which are of the form

$$\Delta'(I0)=\eta f(\Delta(I0))+O(\eta^2). \tag{A1}$$

If we use RPA values as input, $f(\Delta(I0))=\Delta(I0)$, and thus the multiplication by η does not change anything if we make the convention that the RPA amplitudes obtained from the output should all be divided by η. The second term in (A1) can be neglected if η is chosen to be small enough. In the same way, we divide all terms of second order (according to the RPA) by η^2. For example, ω_I' should be of the form

$$\omega_I'=\eta^2\omega_I+O(\eta^3), \tag{A2}$$

where ω_I is the value we use as input. On the contrary, those terms which are of zeroth order, as, e.g., $\Delta(00)$, will come out unchanged, so that no division is necessary. The method then consists in starting the iteration process with a sufficiently small value of η. We first get the self-consistency with that value of η, and then increase η slowly. How slowly η has to be increased depends on the problem at hand. In the example of this paper, we start with $\eta=0.10$ and then increase it by steps of 0.01.

Another point has to be mentioned. The difference between the diagonal elements of (4.9) are of order η^2 while the nondiagonal elements are of order η. Thus, even though the intrinsic off-diagonal elements are small, they may become larger than the differences between the diagonal ones when η is small enough, namely, at the beginning of the iteration. Care has to be taken in this case to avoid wild transformations in the diagonalization of (4.9). We may, for example, artificially multiply all nondiagonal elements by η. The final result, of course, will not be affected because at that point $\eta=1$.

This method of iteration has another advantage in that it allows us to pick up the physical states. We use the following criteria, which is quite plausible from a physical viewpoint: that each solution of the self-consistent problem can be obtained from a solution of the RPA in a continuous way.

At the start of the iteration process, when η is small enough, the $2p\times2p$ secular matrix in (2.3) and (2.4) can be approximately considered as p blocks of 2×2 BCS secular matrices along the diagonal. The solutions are of the form

$$E_{av}\simeq\omega_I\pm E_a(\mathrm{BCS}). \tag{A3}$$

We know in this case how to pick up the corresponding physical state. This solution defines at the same time an eigenvector. At the next step of the iteration, the cor-

responding solution differs very little from the previous one, so that it still can be picked up by forming the scalar products of the eigenvector of the preceding iteration with all the $(2p)$ eigenvectors just obtained and choosing the one that has largest overlap. A criteria based on the energies often does not work because these may and do cross one another during the iteration process.

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Antilinear Operators in Hartree-Bogolyubov Theory. I

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Hartree-Bogolyubov (HB) theory is formulated in a basis-independent way, i.e., in terms of linear and antilinear operators acting in the one-particle space. For that purpose, some basic antilinear algebra is presented. The pairing tensor and the pairing potential are shown to represent two antilinear skew-Hermitian operators. The polar factorization of the first of them (the correlation operator $\hat{t}_a$), i.e., $\hat{t}_a=(\hat{\rho}-\hat{\rho}^2)^{1/2}\hat{P}_a$, shows that HB theory has only two variational (trial) operators: the density operator $\hat{\rho}$ and the antilinear pairing operator $\hat{P}_a$ which is defined by the properties $\hat{P}_a{}^+=\hat{P}_a{}^{\dagger 1}=-\hat{P}_a$. These two operators commute. The former is the unique and very well-known variational operator of Hartree-Fock (HF) theory, and the latter represents a new variational freedom typical of HB theory. Most calculations, as for instance the Bardeen-Cooper-Schrieffer (BCS) approximation, restrict this freedom by choosing $\hat{P}_a$ to be the time-reversal operator. The basic dynamical (Euler-Lagrange) equations of HB theory are obtained directly by varying linear and antilinear operators. They are expressed in a compact form, using only commutators and anticommutators of the kinematical and the dynamical operators:

$$\hat{A}_a\equiv[\hat{h},\hat{t}_a]_+-[\hat{\Delta}_a,\hat{\rho}-\tfrac{1}{2}]_+=0,\quad \hat{B}\equiv[\hat{h},\hat{\rho}]_--[\hat{\Delta}_a,\hat{t}_a]_-=0,$$

where Δ_a is the pairing potential and $\hat{h}$ is the one-particle Hamiltonian.

Two identities are found between $\hat{A}_a$ and $\hat{B}$ which turn out to be very useful for obtaining solutions. Symmetries of the trial operators and of the solutions are discussed in great detail, special attention being paid to real HB solutions and their connection with some antiunitary symmetries. Several simple solutions are analyzed: (1) the case where $\hat{\rho}$ is restricted to be a projector, i.e., $\hat{t}_a=0$ (HF case); (2) the case where $\hat{\rho}$ and $\hat{P}_a$ are restricted to commute with a complete set of observables, which determines the eigensubspaces of $\hat{\rho}$, and which, in particular cases of rotational and translational symmetries, fixes $\hat{P}_a$ to be equal to the time-reversal operator (BCS case); and (3) the case where $\hat{P}_a$ is any given symmetry operator of the Hamiltonian.

INTRODUCTION

THE main aims of this work are:

(1) to show how Hartree-Bogolyubov theory[1–3] can be formulated in terms of one-particle operators independently of any particular representation; to show that for such an operator treatment one has to introduce antilinear operators (correlation operator, pairing operator, pairing potential) into the theory, and that these operators are precisely those variational (trial) operators and corresponding dynamical quantities by which Hartree-Bogolyubov theory differs from the more restricted theory of Hartree-Fock (Sec. I);

(2) to derive two basic dynamical equations of Hartree-Bogolyubov theory by varying the one-particle linear and antilinear operators, and to obtain relations between the operators which enter into these equations (Sec. II);

(3) to discuss symmetry properties of the trial operators and the stationary points, as well as of the dynamical operators, paying special attention to the antiunitary symmetries of the Hamiltonian (Secs. III and IV, case 3);

(4) to analyze some solutions of the Hartree-Bogolyubov dynamical equations, using symmetries and the general relations (Sec. IV).

Actually our method was originally planned[4,5] to clarify the nature of approximations which are necessary

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