Linearization of the Pairing Hamiltonian. II*

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(Received 1 November 1967)

A single-intermediate-state (SIS) approximation is developed for dealing with the pairing Hamiltonian. With the aid of this approximation, expressions are obtained for the ground-state energy of an $(n+2)$-particle system in terms of the ground-state wave function of the n-particle system. Results are obtained for excited-state energies in the n- and $(n\pm1)$-particle systems. Numerical comparisons are made with reliable results obtained with other techniques. It is observed that the results obtained from the SIS approximation are quite accurate. The SIS approximation is also used to point out one source of error inherent in the BCS solution of the pairing problem.

I. INTRODUCTION

In an earlier paper, we pointed out[1] some empirical relations which can be used to linearize the pairing Hamiltonian. The purpose of this paper is to deal with the same problem somewhat more systematically. The main feature of our present approach is the use of a single-intermediate-state (SIS) approximation to exhaust sum rules, whenever necessary. We have found that this procedure must be used with some caution as it leads to some obviously incorrect relations as well as accurate results. We have also found that the same matrix elements which are needed for the calculation of the ground state of the $(n+2)$-particle system can also be used to obtain accurate values of the excitation energies of seniority-two states in the n-particle system. The significance of this result is that accurate, number-conserving solutions of the pairing Hamiltonian can be used for such things as moment-of-inertia calculations, with little sacrifice in speed of calculation relative to the BCS method.

In Sec. II, we state the problem and the symbols which we shall use and list some well-known expressions. In Sec. III, we discuss the SIS approximation. In Sec. IV, we deal with the problem of determining the ground state of the $(n+2)$-particle system when the ground state of the n-particle system is known. We also compare the expressions derived here with numerical results obtained from good number-conserving solutions[2] of the pairing Hamiltonian. In Secs. V and VI, we deal with the excited states of the pairing Hamiltonian, again making comparisons with results obtained from our number-conserving solutions[2] of the pairing Hamiltonian.

II. DEFINITIONS

The Hamiltonian which we consider is of the form

$$H=\sum_{k>0}\epsilon_k(a_k^\dagger a_k+a_{-k}^\dagger a_{-k})-\sum_{k,l>0}G_{l,k}b_l^\dagger b_k, \quad (1)$$

where ϵ_k is a single-particle energy, $a_k^\dagger(a_k)$ is a fermion creation (annihilation) operator, and $-k$ denotes the single-particle state which is the time-reversal partner of k. $G_{l,k}$ is a pairing interaction matrix element, and for the purpose of our derivations, there is no need to assume that it is a constant. The symbols $b_l^\dagger(b_l)$ denote pair-creation (annihilation) operators, i.e.,

$$b_l^\dagger=a_l^\dagger a_{-l}^\dagger, \quad b_l=a_{-l}a_l. \quad (2)$$

The operators $a_k^\dagger$ and a_k obey the fermion anticommutation rules

$$\begin{aligned} &a_k^\dagger a_l+a_l a_k^\dagger=\delta_{k,l},\\ &a_k^\dagger a_l^\dagger+a_l^\dagger a_k^\dagger=a_k a_l+a_l a_k=0. \end{aligned} \quad (3)$$

The symbol N_k denotes the number operator for level k,

$$N_k=a_k^\dagger a_k, \quad (4)$$

and obeys the commutation rules

$$[N_k,b_l^\dagger]=[N_{-k},b_l^\dagger]=\delta_{k,l}b_l^\dagger, \quad (5)$$

$$[b_l,N_k]=[b_l,N_{-k}]=\delta_{k,l}b_l. \quad (6)$$

We shall also need the following relations:

$$[b_l,b_k^\dagger]=[1-N_k-N_{-k}]\delta_{k,l}, \quad (7)$$

$$b_k^\dagger N_k=0, \quad (8)$$

$$N_k b_k=0. \quad (9)$$

We shall use the symbol $|\alpha\rangle$ to designate a seniority-zero eigenstate of the $(n+2)$-particle system, $|\alpha_0\rangle$ to denote the ground state of the $(n+2)$-particle system, and $|\beta\rangle$ to denote the ground state of the n-particle system. We also use the notation

$$\langle M\rangle\equiv\langle\beta|M|\beta\rangle \quad (10)$$

to avoid some clutter in our equations. The final set of equations to bear in mind are

$$N_k|\rho\rangle=N_{-k}|\rho\rangle, \quad (11)$$

$$b_k^\dagger b_k|\rho\rangle=N_k|\rho\rangle, \quad (12)$$

$$b_k b_k^\dagger|\rho\rangle=(1-N_k)|\rho\rangle, \quad (13)$$

whenever the level k(or $-k$) is not occupied by an unpaired particle in the state $|\rho\rangle$.

* Based on work performed under the auspices of the U. S. Atomic Energy Commission.
[1] R. R. Chasman, Phys. Rev. 156, 1197 (1967).
[2] R. R. Chasman, Phys. Rev. 134, B279 (1964).

III. SIS APPROXIMATION

It is well known that one can insert a complete set of intermediate states between operators. As an example, we have

$$\langle\alpha|MN|\beta\rangle=\sum_{\gamma}\langle\alpha|M|\gamma\rangle\langle\gamma|N|\beta\rangle, \quad (14)$$

where γ includes all eigenstates of the Hamiltonian. As it stands, Eq. (14) is not very useful in dealing with the pairing problem. However, if we restrict the summation over γ to a single intermediate state, Eq. (14) becomes quite valuable. The nature of the intermediate state $|\gamma\rangle$ depends on the specific operators M and N which are being considered in each instance. The justification for this approximation comes from the results which it yields. In this section, we shall develop the relations obtained with the SIS approximation.

First we consider the number operator N_k, noting

$$\langle N_k\rangle=\langle N_kN_k\rangle=\langle N_k\rangle\langle N_k\rangle+\langle\beta|N_k|\gamma\rangle\langle\gamma|N_k|\beta\rangle \quad (15)$$

or

$$\langle N_k\rangle[1-\langle N_k\rangle]=\langle\beta|N_k|\gamma\rangle\langle\gamma|N_k|\beta\rangle. \quad (16)$$

We also note

$$\langle\beta|N_k|\gamma\rangle=\langle\beta|N_k|\gamma\rangle[\langle N_k\rangle+\langle\gamma|N_k|\gamma\rangle] \quad (17)$$

or

$$\langle\gamma|N_k|\gamma\rangle=1-\langle N_k\rangle, \quad (18)$$

as well as

$$\langle\gamma|1-N_k|\gamma\rangle=1-\langle\gamma|N_k|\gamma\rangle=\langle N_k\rangle. \quad (18')$$

Next, we consider expressions in which two different indices occur. The SIS approximation yields the results

$$\langle\beta|N_k|\gamma\rangle\langle\gamma|N_l|\beta\rangle=\langle N_kN_l\rangle-\langle N_k\rangle\langle N_l\rangle, \quad (19)$$

$$\langle\gamma|N_kN_l|\gamma\rangle=\langle 1-N_kN_l\rangle, \quad (20)$$

and

$$\langle\gamma|N_k(1-N_l)|\gamma\rangle=1-\langle N_k(1-N_l)\rangle. \quad (21)$$

Equation (19) is interesting in that this SIS approximation result might be valid for any one of three different reasons; (1) there is only one intermediate state for which both $\langle\beta|N_k|\gamma\rangle$ and $\langle\beta|N_l|\gamma\rangle$ are nonzero, (2) Eq. (15) is a good approximation for N_k, or (3) Eq. (15) is a good approximation for N_l. We have included Eq. (20) to further emphasize the comment made in the introduction that the SIS approximation must be used with some caution. By combining Eqs. (18) and (20), we obtain the incorrect result

$$\langle\gamma|N_k(1-N_l)|\gamma\rangle=\langle N_kN_l\rangle-\langle N_k\rangle. \quad (21')$$

Equation (21′) is obviously incorrect because diagonal matrix elements of the form

$$(N_jN_k\cdots(1-N_l)(1-N_m)\cdots)$$

must be positive. We can avoid errors of the type of Eq. (21′) by noting that the intermediate state of Eq. (18) is different from that of Eq. (20); one depending on N_k and the other on N_kN_l. Equation (21) is obtained by considering a SIS depending on the total operator $N_k(1-N_l)$.

The next group of expressions to consider are those which involve pair creation and annihilation operators. We first consider

$$\langle\alpha|b_k^\dagger|\gamma\rangle=\langle\alpha|b_k^\dagger(1-N_k)|\gamma\rangle=\langle\alpha|b_k^\dagger|\beta\rangle\langle\beta|(1-N_k)|\gamma\rangle+\langle\alpha|b_k^\dagger|\gamma\rangle\langle\gamma|(1-N_k)|\gamma\rangle \quad (22)$$

or

$$\langle\alpha|b_k^\dagger|\gamma\rangle=\langle\alpha|b_k^\dagger|\beta\rangle\langle\beta|(1-N_k)|\gamma\rangle/(1-\langle N_k\rangle), \quad (23)$$

where we have used Eq. (18).

Next, we consider the expression $\langle\beta|b_k^\dagger b_l|\gamma\rangle$, noting

$$\langle\beta|b_k^\dagger b_l|\gamma\rangle=\langle\beta|b_k^\dagger b_lN_l(1-N_k)|\gamma\rangle, \quad (24)$$

from which we obtain via the SIS approximation

$$\langle\beta|b_k^\dagger b_l|\gamma\rangle=\frac{\langle b_k^\dagger b_l\rangle}{\langle N_l(1-N_k)\rangle}\langle\beta|N_l(1-N_k)|\gamma\rangle. \quad (25)$$

The procedure implicit in the derivations of Eqs. (23) and (25) is to insert a factor of $(1-N_g)$ for every pair-creation operator $b_g^\dagger$ and a factor N_g for every pair-annihilation operator b_g in such a way that the value of the expression is unchanged. When the intermediate state appears to the left as $\langle\gamma|$, N_j is inserted to the left of pair-creation operators $b_j^\dagger$ and $(1-N_j)$ to the left of pair-annihilation operators b_j. We then assume that the intermediate state populated by the product of pair-creation and -annihilation operators is the same state $|\gamma\rangle$ which obeys a relation of the type of Eq. (15) for the product $(N_gN_k\cdots(1-N_l)(1-N_m)\cdots)$ obtained in this way. We shall encounter cases in which the operators to the left of $|\gamma\rangle$ suggest a different choice of SIS from those to the right of $\langle\gamma|$. In those cases, we use one of the two products of number operators to define the SIS $|\gamma\rangle$ (or $\langle\gamma|$).

Equation (25) is of interest in that it can be used to obtain the BCS equations. We start from the observation

$$\langle N_k(1-N_l)\rangle=\langle b_k^\dagger b_lb_l^\dagger b_k\rangle=\langle b_k^\dagger b_l\rangle^2+\langle\beta|b_k^\dagger b_l|\gamma\rangle\langle\gamma|b_l^\dagger b_k|\beta\rangle, \quad (26)$$

where we have used

$$\langle b_k^\dagger b_l\rangle=\langle b_l^\dagger b_k\rangle. \quad (27)$$

Introducing Eq. (25) into Eq. (26), we soon obtain the relations

$$\langle b_k^\dagger b_l\rangle=[\langle N_k(1-N_l)\rangle\langle N_l(1-N_k)\rangle]^{1/2}. \quad (28)$$

If we make the additional approximation

$$\langle N_kN_l\rangle\approx\langle N_k\rangle\langle N_l\rangle \quad (29)$$

and substitute Eqs. (28) and (12) into Eq. (1), the BCS equations are obtained by first putting the term

$-\lambda\sum_k\langle N_k\rangle$ into the Hamiltonian and then setting

$$\partial H/\partial\langle N_k\rangle=0 \quad \text{for all } \langle N_k\rangle. \tag{30}$$

Equation (28) is an excellent approximation (in fact, it would be exact if the eigenfunctions of the pairing Hamiltonian had separable[2] amplitudes) so from the point of view of the SIS approximation, we may argue that one of the problems of the BCS method arises from the rather poor approximation of Eq. (29). It is unfortunate that the SIS approach does not seem to yield any reasonable approximation for the expression $\langle N_kN_l\rangle$.

The final result of the SIS approximation, which we shall need in Sec. IV, is

$$\langle\alpha|b_k^\dagger|\beta\rangle\langle N_k\rangle=-\langle\alpha|b_k^\dagger|\gamma\rangle\langle\gamma|N_k|\beta\rangle, \tag{31}$$

which follows directly from Eq. (8).

IV. EIGENSTATES OF THE $(n+2)$-PARTICLE SYSTEM

The assumption which we make here is that we have in some way[2] obtained a wave function $|\beta\rangle$, the ground state of an n-particle system. We then compute the matrix elements $\langle b_k^\dagger b_l\rangle$, $\langle N_k\rangle$, and $\langle N_kN_l\rangle$ directly. The problem is to determine states $|\alpha\rangle$ in the $(n+2)$-particle system. To this end, we take the commutator of $b_k^\dagger$ with the Hamiltonian of Eq. (1) and obtain

$$[H,b_k^\dagger]=2\epsilon_kb_k^\dagger-\sum_{l>0}G_{l,k}b_l^\dagger(1-2N_k). \tag{32}$$

When we evaluate Eq. (32) between states $|\alpha\rangle$ and $|\beta\rangle$ we have

$$[2\epsilon_k-(E_\alpha-E_\beta)]\langle\alpha|b_k^\dagger|\beta\rangle=\sum_{l>0}G_{l,k}\langle\alpha|b_l^\dagger|\beta\rangle -\sum_{l>0}2G_{l,k}\langle\alpha|b_l^\dagger N_k|\beta\rangle, \tag{33}$$

where we have used the notation

$$E_\nu=\langle\nu|H|\nu\rangle. \tag{34}$$

The difficulty is to determine $\langle\alpha|b_l^\dagger N_k|\beta\rangle$ as some general expansion of the form

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\sum_{m,n}D(l,k;m,n)\langle\alpha|b_m^\dagger|\beta\rangle\langle R_n\rangle. \tag{35}$$

If we can derive expressions of the form of Eq. (35), the eigenvalue E_α can be readily obtained from Eq. (33). In fact, we shall find expressions considerably simpler to use than is suggested by Eq. (35). To this end, we multiply Eq. (32) from the right by N_k, which gives the result

$$-b_k^\dagger HN_k=\sum_{l>0}G_{l,k}b_l^\dagger N_k \tag{36}$$

using Eq. (8). Using the SIS approximation for the left side of Eq. (36) and also making use of Eq. (31) we have

$$(E_{\gamma_k}-E_\beta)\langle\alpha|b_k^\dagger|\beta\rangle\langle N_k\rangle=\sum_{l>0}G_{l,k}\langle\alpha|b_l^\dagger N_k|\beta\rangle \tag{37}$$

and the problem is to determine E_{γ_k}. To do this, we multiply Eq. (36) from the left by b_k and obtain

$$-(1-N_k)HN_k=\sum_{l>0,l\neq k}G_{l,k}b_l^\dagger b_k. \tag{38}$$

After applying the SIS approximation to the left side of Eq. (38) and making use of Eq. (16), we obtain the relation

$$(E_{\gamma_k}-E_\beta)\langle N_k\rangle[1-\langle N_k\rangle]=\sum_{l>0,l\neq k}G_{l,k}\langle b_l^\dagger b_k\rangle. \tag{39}$$

Finally, we combine Eq. (39) with Eq. (37) and have the desired result

$$\sum_{l>0}G_{l,k}\langle\alpha|b_l^\dagger N_k|\beta\rangle=\frac{\langle\alpha|b_k^\dagger|\beta\rangle}{1-\langle N_k\rangle}\sum_{l>0,l\neq k}G_{l,k}\langle b_l^\dagger b_k\rangle. \tag{40}$$

In the series of steps leading to Eq. (40) there is no ambiguity in the definition of the SIS $|\gamma\rangle$. From this derivation of Eq. (40), we conclude that the proper intermediate state to be used in the evaluation of $\langle\alpha|b_l^\dagger N_k|\beta\rangle$ is the state discussed in Eqs. (15)–(18). With this point in mind, we can obtain the results of Eq. (40) in a different and simpler way. We start with the relation

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\langle\alpha|b_l^\dagger b_k^\dagger b_k|\beta\rangle=\langle\alpha|b_k^\dagger b_l^\dagger b_k|\beta\rangle \tag{41}$$

and continuing to manipulate this expression, we obtain

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\langle\alpha|b_k^\dagger|\beta\rangle\langle b_l^\dagger b_k\rangle +\langle\alpha|b_k^\dagger|\gamma\rangle\langle\gamma|b_l^\dagger b_k|\beta\rangle. \tag{42}$$

For the intermediate state $|\gamma\rangle$ determined by the operator $(1-N_k)$, we may substitute Eq. (23) into Eq. (42), and this leads directly to the relation,

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=[\langle\alpha|b_k^\dagger|\beta\rangle/(1-\langle N_k\rangle)]\langle b_l^\dagger b_k\rangle, \tag{43}$$

which is equivalent to Eq. (40), bearing in mind Eq. (8).

We should, however, expect that the SIS $|\gamma\rangle$ depends on both $b_l^\dagger$ and N_k. This expectation leads us to write

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\langle\alpha|b_k^\dagger N_lb_l^\dagger b_k|\beta\rangle, \tag{44}$$

which we expand as

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\langle\alpha|b_k^\dagger N_l|\beta\rangle\langle b_l^\dagger b_k\rangle +\langle\alpha|b_k^\dagger N_l|\gamma\rangle\langle\gamma|b_l^\dagger b_k|\beta\rangle. \tag{45}$$

Substituting Eq. (25) into Eq. (45), we obtain the result

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\langle\alpha|b_k^\dagger N_l|\beta\rangle\langle b_l^\dagger b_k\rangle/\langle N_l(1-N_k)\rangle. \tag{46}$$

As the SIS used in obtaining Eq. (46) is somewhat more intuitively satisfying than the SIS which is used to obtain Eq. (40) or Eq. (43), we might expect Eq.

Eq. (46) to be the better approximation. To anticipate, comparison with numerical results indicates that Eq. (46) is an excellent approximation [about as good as Eq. (28)]. However, Eq. (46) does not linearize our problem; it is rather approximations of the form of Eq. (43) which we need.

Equations (46), (43), and (28) taken together give an additional approximation for $\langle\alpha|b_l^\dagger N_k|\beta\rangle$, which is

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=[\langle\alpha|b_l^\dagger|\beta\rangle/(1-\langle N_l\rangle)]\langle N_k(1-N_l)\rangle. \quad (47)$$

Equation (47) can be obtained directly by assuming that the appropriate SIS approximation is determined by the operator $(1-N_l)$. This can be seen by writing

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=\langle\alpha|b_l^\dagger|\beta\rangle\langle N_k(1-N_l)\rangle +\langle\alpha|b_l^\dagger|\gamma\rangle\langle\gamma|N_k(1-N_l)|\beta\rangle \quad (48)$$

and substituting from Eq. (23) for $\langle\alpha|b_l^\dagger|\gamma\rangle$.

At this point, we have two approximations for the matrix element $\langle\alpha|b_l^\dagger N_k|\beta\rangle$, which are of the form of Eq. (35). The result of Eq. (43) is obtained by assuming that the properties of the SIS $|\gamma\rangle$ are determined by the operator $(1-N_k)$ and the result of Eq. (47) is obtained by assuming that the properties of the SIS are determined by the operator $(1-N_l)$. These are the only approximations for $\langle\alpha|b_l^\dagger N_k|\beta\rangle$ of the form of Eq. (35) which we have been able to derive with the SIS approximation. It should be noted that either approximation is better than the usual one of ignoring intermediate-state effects.

We might hope that there exists some linear combination of Eqs. (43) and (47) which gives a better approximation for $\langle\alpha|b_l^\dagger N_k|\beta\rangle$ than either equation used by itself. *A priori*, there is little basis for determining the appropriate linear combination for each choice of l and k. We can, however, compare the approximations with some numerical results in order to deduce appropriate linear combinations. Before resorting to the examination of numerical results, however, we shall make some use of Eq. (46). Let us assume that we have a relation of the form

$$\langle\alpha|b_k^\dagger N_l|\beta\rangle=A_{k,l}\frac{\langle\alpha|b_k^\dagger|\beta\rangle}{1-\langle N_k\rangle}\langle N_l(1-N_k)\rangle +(1-A_{k,l})\frac{\langle\alpha|b_l^\dagger|\beta\rangle}{1-\langle N_l\rangle}\langle b_k^\dagger b_l\rangle. \quad (49)$$

We can then use Eq. (46) to obtain a relation for $\langle\alpha|b_l^\dagger N_k|\beta\rangle$ in terms of the same coefficient $A_{k,l}$. If we substitute Eq. (49) into Eq. (46), bearing in mind Eq. (28), we obtain

$$\langle\alpha|b_l^\dagger N_k|\beta\rangle=A_{k,l}\frac{\langle\alpha|b_k^\dagger|\beta\rangle}{1-\langle N_k\rangle}\langle b_l^\dagger b_k\rangle +(1-A_{k,l})\frac{\langle\alpha|b_l^\dagger|\beta\rangle}{1-\langle N_l\rangle}\langle N_k(1-N_l)\rangle. \quad (50)$$

TABLE I. Evaluation of $\langle\alpha|b_l^\dagger N_k|\beta\rangle$.

$N_k>N_l$	
$N_k>0.5$[a] $\dfrac{\langle\alpha\|b_l^\dagger\|\beta\rangle\langle N_k(1-N_l)\rangle}{1-\langle N_l\rangle}$	$N_k<0.5$ $\dfrac{\langle\alpha\|b_k^\dagger\|\beta\rangle\langle b_l^\dagger b_k\rangle}{1-\langle N_k\rangle}$
$N_l>N_k$	
$N_l>0.5$[a] $\dfrac{\langle\alpha\|b_k^\dagger\|\beta\rangle\langle b_l^\dagger b_k\rangle}{1-\langle N_k\rangle}$	$N_l<0.5$ $\dfrac{\langle\alpha\|b_l^\dagger\|\beta\rangle\langle N_k(1-N_l)\rangle}{1-\langle N_l\rangle}$

[a] By $N_k>0.5$, we mean somewhat more precisely that level k is occupied in the limit $G\to 0$.

The need to satisfy Eqs. (49) and (50) simultaneously sharply limits the choices of coefficients $A_{k,l}$. At this point, we are ready to use the results of direct evaluations. For this purpose, we have used wave functions of a system in which there are 16 equally spaced levels. We have also chosen $G_{k,l}=G$, as we believe that we can best calculate[2] wave functions for the constant G interaction. We have chosen G as one-half the single-particle spacing and seven pairs for the $|\beta\rangle$ system, with eight pairs of particles for the $|\alpha\rangle$ system. With these wave functions we have computed directly the quantities $\langle\alpha_0|b_l^\dagger N_k|\beta\rangle$, $\langle\alpha_0|b_l^\dagger|\beta\rangle$, $\langle b_k^\dagger b_l\rangle$, and $\langle N_k N_l\rangle$, where $|\alpha_0\rangle$ denotes the ground state of the eight-pair-system. Bearing in mind the restrictions imposed by Eqs. (49) and (50), we conclude that it is a good approximation to assume that $A_{k,l}$ is either 0 or 1. In Table I, we present the approximation for $\langle\alpha_0|b_l^\dagger N_k|\beta\rangle$ which we have deduced from a direct comparison. In Fig. 1, we examine the ratio of $\sum_l\langle\alpha_0|b_l^\dagger N_k|\beta\rangle$ to the approximation of Table I as well as to the approximation of Eq. (40). It may be of some interest to compare this ratio to those plotted in Fig. 1, Ref. 1. Note that the approximation of Eq. (40) is also fairly good; it is at its worst as $N_k\to 0$ and $\langle\alpha|b_l^\dagger N_k|\beta\rangle$ is not too

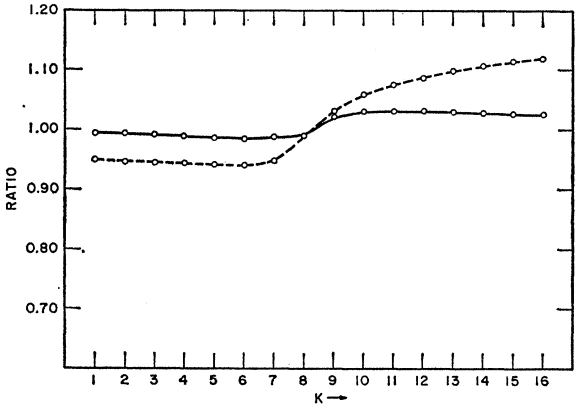

FIG. 1. Ratio of $\sum_l\langle\alpha|b_l^\dagger N_k|\beta\rangle$ to various approximations. The solid curve gives the ratio with respect to the approximation of Table I; the dashed curve, with respect to the right-hand side of Eq. (40).

important on the right-hand side of Eq. (33). The advantage of using Eq. (40) relative to Table I is that it leads to some simple equations. Substituting Eq. (40) back into Eq. (33), we have

$$\left[2\epsilon_k-(E_{\alpha_0}-E_\beta)+2\sum_{l>0,l\neq k}G_{l,k}\frac{\langle b_l^\dagger b_k\rangle}{1-\langle N_k\rangle}\right]\langle\alpha_0|b_k^\dagger|\beta\rangle=\sum_{l>0}G_{l,k}\langle\alpha_0|b_l^\dagger|\beta\rangle \quad (51)$$

which, in the case of constant $G_{l,k}$, yields the simple eigenvalue equation

$$1=G\sum_k\left(2\epsilon_k+2G\sum_{l\neq k,l>0}\frac{\langle b_l^\dagger b_k\rangle}{1-\langle N_k\rangle}-(E_{\alpha_0}-E_\beta)\right)^{-1}. \quad (52)$$

Equation (52), together with some iterative procedure of the type developed by Giu and Klein,[3] might be developed as a SIS approximation, as easy to use as the BCS approximation, and having no problems of number conservation or trivial solutions. There are some difficulties.

The next question to consider is that of seniority-zero excited states $|\alpha\rangle$. We conclude that the linear combination appropriate to $|\alpha_0\rangle$ cannot be appropriate for these states in a strict sense. The starting point for this conclusion is the relation

$$\langle N_l(1-N_k)\rangle=\langle N_l b_k b_k^\dagger\rangle=\langle b_k b_k^\dagger N_l\rangle. \quad (53)$$

We rewrite Eq. (53) as

$$\langle N_l(1-N_k)\rangle=\sum_{|\alpha>}\langle\beta|b_k|\alpha\rangle\langle\alpha|b_k^\dagger N_l|\beta\rangle \quad (54)$$

and let us assume that $\langle N_k\rangle$ and $\langle N_l\rangle$ are such that

$$\langle\alpha_0|b_k^\dagger N_l|\beta\rangle=\frac{\langle\alpha_0|b_l^\dagger|\beta\rangle}{1-\langle N_l\rangle}\langle b_k^\dagger b_l\rangle, \quad (55)$$

according to Table I.

Combining Eqs. (54), (55), and (28) we obtain the result, if (55) holds for all states $\langle\alpha|$,

$$1=\langle N_k(1-N_l)\rangle/(1-\langle N_l\rangle), \quad (56)$$

which is obviously incorrect. The problem of seniority-zero excited states is still to be solved in the SIS approximation, but the ground-state problem is solved.

V. SENIORITY-TWO EXCITED STATES OF THE N-PARTICLE SYSTEM

The problem to be dealt with in this section is: Given an eigenfunction $|\beta\rangle$, what can be said about the seniority-two excited states? We shall consider the excited state in which levels r and t are blocked. Taking the commutator of $a_r^\dagger a_{-t}$ with the Hamiltonian, we obtain

$$[H,a_r^\dagger a_{-t}]=(\epsilon_r-\epsilon_t)a_r^\dagger a_{-t}-\sum_k G_{k,r}b_k^\dagger a_{-r}a_{-t}-\sum_k G_{t,k}a_r^\dagger a_t^\dagger b_k. \quad (57)$$

Multiplication of Eq. (57) from the left by $a_{-t}^\dagger a_r$ gives

$$a_{-t}^\dagger a_r[H,a_r^\dagger a_{-t}]=(\epsilon_r-\epsilon_t)N_{-t}(1-N_r)+\sum_{k\neq r,t}G_{k,r}b_k^\dagger b_r N_{-t}+\sum_k G_{t,k}b_t^\dagger(1-N_r)b_k \quad (58)$$

and multiplication of (57) from the left by $a_t a_{-r}^\dagger$ gives

$$a_t a_{-r}^\dagger[H,a_r^\dagger a_{-t}]=(\epsilon_r-\epsilon_t)b_r^\dagger b_t+\sum_{k\neq r,t}G_{k,r}b_k^\dagger b_t(N_{-r})+\sum_k G_{t,k}b_r^\dagger(1-N_t)b_k. \quad (59)$$

Two more equations can be obtained by interchanging the indices r and t in Eqs. (58) and (59). When we evaluate these equations for $|\beta\rangle$ we get terms of the form $\sum_\gamma\langle\beta|a_{-t}^\dagger a_r|\gamma\rangle E_\gamma\langle\gamma|a_r^\dagger a_{-t}|\beta\rangle$, which are to be evaluated in terms of the SIS approximation. This time there are two related sum rules to consider, and hence two intermediate states to deal with.

The first sum rule to consider is

$$\langle N_{-t}(1-N_r)\rangle=\langle\beta|a_{-t}^\dagger a_r|\gamma\rangle\langle\gamma|a_r^\dagger a_{-t}|\beta\rangle+\langle\beta|a_{-t}^\dagger a_r|\delta\rangle\langle\delta|a_r^\dagger a_{-t}|\beta\rangle, \quad (60)$$

where $|\delta\rangle$ represents the contribution to the sum rule of all seniority-two excited states other than the lowest one, $|\gamma\rangle$, in which we are interested. The second sum rule to consider comes from the normalization of $|\gamma\rangle$, i.e.,

$$1=\langle\gamma|a_r^\dagger a_{-t}a_{-t}^\dagger a_r|\gamma\rangle \quad (61)$$

or

$$1=\langle\gamma|a_r^\dagger a_{-t}|\beta\rangle\langle\beta|a_{-t}^\dagger a_r|\gamma\rangle+\langle\gamma|a_r^\dagger a_{-t}|\eta\rangle\langle\eta|a_{-t}^\dagger a_r|\gamma\rangle, \quad (62)$$

where $|\eta\rangle$ is a seniority-zero intermediate state. As $|\delta\rangle$ is orthogonal to $|\gamma\rangle$ in the paired part of its wave function,

$$\langle\gamma|a_r^\dagger a_{-t}a_{-t}^\dagger a_r|\delta\rangle=0 \quad (63)$$

or

$$\langle\gamma|a_r^\dagger a_{-t}|\beta\rangle\langle\beta|a_{-t}^\dagger a_r|\delta\rangle+\langle\gamma|a_r^\dagger a_{-t}|\eta\rangle\langle\eta|a_{-t}^\dagger a_r|\delta\rangle=0. \quad (64)$$

Next, we note

$$\langle\gamma|a_r^\dagger a_{-t}|\eta\rangle=\langle\gamma|a_r^\dagger a_{-t}N_{-t}(1-N_r)|\eta\rangle \quad (65)$$

and, in the usual way, we obtain

$$\langle\gamma|a_r^\dagger a_{-t}|\eta\rangle=\frac{\langle\gamma|a_r^\dagger a_{-t}|\beta\rangle}{\langle N_{-t}(1-N_r)\rangle}\langle\beta|N_{-t}(1-N_r)|\eta\rangle. \quad (66)$$

Substituting Eq. (66) into Eq. (64) and doing a little

[3] D. D. Giu and A. Klein, Phys. Rev. 143, 735 (1966).

manipulation gives us the result

$$\langle\gamma|a_r^\dagger a_{-t}|\beta\rangle\langle\beta|a_{-t}^\dagger a_r|\delta\rangle=0 \tag{67}$$

or

$$\langle\beta|a_{-t}^\dagger a_r|\delta\rangle=0. \tag{68}$$

Equation (68) means that in the SIS approximation there is no coupling between the ground state and seniority two-pairing excited states. Now, we return to Eqs. (58), (59), and the two equations to be obtained from them by interchanging indices. We evaluate the four equations for the state $|\beta\rangle$, and combine them to get the result of interest:

$$(E_\gamma^{r,t}-E_\beta)=\frac{(\epsilon_r-\epsilon_t)[\langle N_t\rangle-\langle N_r\rangle]}{\langle N_r(1-N_t)\rangle+\langle N_t(1-N_r)\rangle-2\langle b_r^\dagger b_t\rangle} \tag{69}$$

in the case of $G_{l,m}$ being a constant, and in general we have

$$\begin{aligned}[E_\gamma^{r,t}-E_\beta]=D[&(\epsilon_r-\epsilon_t)(\langle N_t\rangle-\langle N_r\rangle)\\&+(G_{t,t}-G_{r,t})(\langle N_t(1-N_r)\rangle-\langle b_r^\dagger b_t\rangle)]\\&+D[(G_{r,r}-G_{r,t})(\langle N_r(1-N_t)\rangle-\langle b_r^\dagger b_t\rangle)]\\&+D\sum_{k\neq r,t}(G_{r,k}-G_{t,k})(\langle b_r^\dagger b_k\rangle-\langle b_t^\dagger b_k\rangle),\end{aligned} \tag{70}$$

with

$$D=[\langle N_r(1-N_t)\rangle+\langle N_t(1-N_r)\rangle-2\langle b_r^\dagger b_t\rangle]^{-1}. \tag{70'}$$

We have tested Eq. (69), with a system of 16 particles in 16 equally spaced levels ($G=200$ keV, $\Delta\epsilon=400$ keV) and present the results in Table II. From Table II, it can be seen that Eq. (69) appears to be an extremely good approximation; we find this agreement somewhat surprising. We also note in Table II that the discrepancies are largest when both levels r and t are both on the same side of and far from the Fermi surface. In these cases, there is a better approximation. Let us assume that both levels are far above the Fermi surface (i.e., $N_r\to 0$, $N_t\to 0$). It is then clear that the pairing part of the seniority-two excited state should be almost the same as the ground state of the $(n-2)$- (in this case 14) particle system and the appropriate quantity to consider is $\langle a_r a_t[H,a_r^\dagger a_t^\dagger]\rangle$, where the brackets indicate the seven-pair ground state. The expression which we obtain is

$$\begin{aligned}(E_\gamma^{r,t}-E_\beta)=(\epsilon_r+\epsilon_t)&+\frac{\sum_{k\neq r,t}G_{k,r}\langle b_k^\dagger b_r(1-N_t)\rangle}{\langle(1-N_r)(1-N_t)\rangle}\\&+\sum_{k\neq r,t}G_{k,t}\frac{\langle b_k^\dagger b_t(1-N_r)\rangle}{\langle(1-N_r)(1-N_t)\rangle}.\end{aligned} \tag{71}$$

As $\langle N_r\rangle$ and $\langle N_t\rangle$ are quite small by assumption we do not get into any trouble setting

$$\langle b_k^\dagger b_r N_t\rangle=\langle b_k^\dagger b_r\rangle\langle N_t\rangle \tag{72}$$

TABLE II. Energies of seniority-two states.

Blocked levels[a]	Excitation energy (MeV)[b]	Excitation energy, Eq. (69) (MeV)[c]
(1,2)	6.48	6.71
(1,6)	4.98	5.12
(1,8)	4.32	4.38
(1,10)	4.32	4.35
(1,15)	6.10	6.08
(5,1)	5.35	5.51
(5,6)	3.45	3.55
(5,8)	2.78	2.83
(5,10)	2.79	2.80
(5,15)	4.60	4.60
(8,1)	4.32	4.38
(8,5)	2.78	2.83
(8,7)	2.06	2.09
(8,9)	1.47	1.47
(8,11)	2.16	2.18
(8,15)	3.68	3.73
(9,1)	4.07	4.13
(9,5)	2.53	2.57
(9,7)	1.80	1.81
(9,8)	1.47	1.47
(9,10)	2.06	2.07
(9,11)	2.41	2.43
(11,1)	4.63	4.64
(11,5)	3.12	3.12
(11,7)	2.43	2.43
(11,9)	2.41	2.43
(11,15)	4.59	4.75
(16,1)	6.48	6.46
(16,5)	4.98	4.98
(16,7)	4.32	4.35
(16,9)	4.32	4.38
(16,14)	6.10	6.38

[a] The two numbers in the first column show which two levels of the system are blocked.
[b] The second column gives the excitation energy as calculated with the methods of Ref. 2.
[c] The third column gives the excitation energy calculated with Eq. (69).

and this approximation reduces the errors in Table II considerably for such cases. When both levels are below the Fermi surface, we start with the ground state of the $(n+2)$-particle system.

VI. SENIORITY-ONE STATES OF THE $(n+1)$-PARTICLE SYSTEM

We here use the symbol $|\alpha_K\rangle$ to denote the seniority-one eigenstate in the $(n+1)$-particle system, $|\beta\rangle$ the ground state of the n-particle system, and $|\beta'\rangle$ the ground state of the $(n+2)$-particle system. Taking the commutator of $a_K^\dagger$ with the Hamiltonian to obtain the relation

$$\begin{aligned}(E_{\alpha K}-E_\beta)\langle\alpha_K|a_K^\dagger|\beta\rangle&=\epsilon_K\langle\alpha_K|a_K^\dagger|\beta\rangle\\&\quad-\sum_{l>0}G_{l,K}\langle\alpha_K|b_l^\dagger a_{-K}|\beta\rangle,\end{aligned} \tag{73}$$

and also noting

$$\langle\alpha_K|b_l^\dagger a_{-K}|\beta\rangle=-\langle\alpha_K|a_K^\dagger b_l^\dagger b_K|\beta\rangle, \tag{74}$$

TABLE III. Energies of seniority-one states.

Blocked level	$E_{\alpha K}-E_\beta$(MeV) Eq. (75)	$E_{\alpha K}-E_\beta$(MeV) Eq. (76′)	$E_{\alpha K}-E_\beta$(MeV) Direct[a]
1	6.831	6.551	6.552
2	6.436	6.165	6.166
3	6.040	5.783	5.783
4	5.643	5.405	5.405
5	5.247	5.035	5.033
6	4.855	4.676	4.672
7	4.471	4.336	4.328
8	4.108	4.033	4.016
9	3.825	3.825	3.781
10	4.028	4.105	4.012
11	4.327	4.478	4.320
12	4.665	4.867	4.662
13	5.023	5.263	5.021
14	5.393	5.657	5.392
15	5.770	6.047	5.770
16	6.152	6.433	6.152

[a] See Ref. 2.

we soon derive

$$E_{\alpha K}=E_\beta+\epsilon_K+\sum_{l\neq K,l>0}\frac{G_{l,K}\langle b_l^\dagger b_K\rangle}{1-\langle N_K\rangle} \tag{75}$$

with the aid of the SIS approximation. A similar set of steps yields the second relation

$$E_{\alpha K}=E_{\beta'}-\epsilon_K+G_{K,K}+\sum_{l\neq K,l>0}G_{l,K}\frac{\langle\beta'|b_K^\dagger b_l|\beta'\rangle}{\langle\beta'|N_K|\beta'\rangle}. \tag{76}$$

The SIS approximation also gives the results

$$\langle\alpha_K|a_K^\dagger|\beta\rangle^2=1-\langle N_K\rangle \tag{77}$$

and

$$\langle\alpha_K|a_{-K}|\beta'\rangle^2=\langle\beta'|N_K|\beta'\rangle. \tag{78}$$

In Table III, we test Eqs. (75) and (76) for the case of constant $G_{l,K}$ (again 16 levels, $\Delta\epsilon=400$ keV and $G=200$ keV.) Here, we have chosen $n=16$. In order to facilitate comparisons we have used

$$E_{\alpha K}-E_\beta=E_{\beta'}-E_\beta+G+G\sum_{l\neq K,l>0}\frac{\langle\beta'|b_K^\dagger b_l|\beta'\rangle}{\langle\beta'|N_K|\beta'\rangle} \tag{76′}$$

in the construction of Table III. As would be expected from Eqs. (77) and (78), Table III indicates that Eq. (75) is better for particle states and Eq. (76) is better for hole states. Table III also indicates that we have an extremely quick and accurate way to obtain complete spectra of seniority-one states in a given nucleus.

VII. CONCLUSIONS AND COMMENTS

The main conclusion to be drawn from this work is that the SIS method is an appropriate one to use in the treatment of pairing interactions. The evidence for this conclusion comes from Secs. IV–VI of this paper; specifically, from Fig. 1 and Tables II and III. We feel that this procedure will prove to be valuable in dealing with other two-body interactions, as it is a natural approximation to make in the application of second quantization techniques.

The results of Secs. V and VI suggest methods for dealing with residual interactions, using only ground-state wave functions. The open problem is the calculation of the ground-state wave function with the SIS approximation. The stumbling block is the evaluation of two-pair correlations $\langle N_kN_l\rangle$ in terms of occupation probabilities $\langle N_k\rangle$ and $\langle N_l\rangle$.

The various intermediate states which arise in the application of the SIS method should be regarded as an average of many excited states. It is somewhat surprising and extremely gratifying that the SIS procedure handles effects due to the excited-state spectrum so well.

ACKNOWLEDGMENTS

It is a pleasure to thank D. Kurath for a careful reading of this manuscript and D. D. Giu for a useful discussion of this problem.