Nucleon-number-conserving description of pairing correlations in terms of occupation probability amplitudes

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A practical number-conserving method of treating pairing correlations is proposed. The theory is formulated in a form having clear correspondence with quasiparticle theory and, moreover, it works well even in the weak pairing limit. Various matrix elements are approximately expressed in terms of the occupation probabilities containing the blocking effects within the number-conserving framework. The exact occupation probabilities can be used in the case of a constant pairing force. The present method is able to take the place of previous fixed-number BCS methods and is suitable for treating residual correlations further. Application to the cranking model is discussed.

I. INTRODUCTION

The treatment of pairing correlations has been a matter of concern in the microscopic study of nuclear collective motions. We refer to only a few recent papers,[1-3] although numerous papers[4] have discussed the pairing problem. The aim beyond the pairing problem is to deal with other residual correlations. The treatment of the pairing degree of freedom should be suitable for this further step. The simplest method to use is the Bardeen-Cooper-Schrieffer (BCS) quasiparticle or the Hartree-Fock-Bogoliubov (HFB) approach. However, its disadvantage is nonconservation of nucleon number and it is not good in weak pairing situations. For instance, recent calculations with the fixed-number BCS (FBCS) (Refs. 5 and 6) have revealed that the simple HFB does not necessarily succeed in high-spin states of deformed nuclei. Many efforts[1-4] have been made to restore the number conservation but only a few methods are simple enough to apply to general cases. The usual fixed-number methods are not useful enough for calculation of matrix elements when we deal with residual correlations.

The purpose of this paper is to develop a practical number-conserving treatment of the pairing degree of freedom and to give an approximate method of evaluating various matrix elements even for excited states in this number-conserving treatment.

Our basic approximation is to describe the pairing correlated states in a number-conserving form by using the occupation probabilities V_ν^2. This allows us to express the contributions of the pairing degree of freedom to various matrix elements in terms of V_ν^2. The idea is similar to the approaches of Li[1] and Lorazo and Quesne,[2] who start with the FBCS wave functions. We discuss the connection in Sec. IV. The present approach is completed when the coefficients V_ν^2 are determined by a number-conserving treatment of the pairing correlations appropriate for each problem. We can use the exact V_ν^2 in the case of constant pairing force (and also in spherical nuclei) and otherwise the approximate V_ν^2 obtained by the FBCS.

The problem of treating the blocking effects[7,8] is difficult for the quasiparticle theory, because the effects introduce different quasiparticle bases.[9] On the other hand, our theory is able to take account of the blocking effects in a proper way. The unpaired degrees of freedom separated from the pairing one are expressed in terms of operators like quasiparticles. The treatment, therefore, preserves clear correspondence with the quasiparticle treatment and is suitable for dealing with residual correlations.

The present method is superior to the BCS quasiparticle approach. In the superconducting case, the approximation gives results better than the BCS even if we use V_ν^2 obtained by the BCS equations. It is still more applicable to weak pairing situations where the BCS equations do not work. Moreover, the evaluation of various matrix elements is very easy. The method is expected to be applicable to many problems in which the BCS approximation is not good.

In Sec. II we present a new formalism describing the pairing correlations and give our basic approximation for the pairing eigenstates. In Sec. III we explain how to evaluate various matrix elements and energies. An easy way to determine V_ν^2 in the superconducting case is also shown. In Sec. IV the present method is discussed and compared with other approaches. We examine our basic approximation in a model where we can use the exact V_ν^2. Application to the cranking model is discussed in Sec. V.

II. APPROXIMATION FOR THE PAIRING EIGENSTATES

A. Separation of the pairing degree of freedom from the others

We start with a consideration of the nucleon operators $(c_{\nu\sigma}^\dagger, c_{\nu\sigma})$ in a certain self-consistent field. Let us regard appropriate couples of single-particle states as "conjugate" states and distinguish each pair of conjugate states by the subscript σ ($+$ or $-$). (For instance, σ means the signa-

ture in a time-reversal symmetric basis.) Using the Pauli exclusion principle $c^\dagger_{\nu\sigma}c^\dagger_{\nu\sigma}=0$, we obtain the equality

$$c^\dagger_{\nu\sigma}=c^\dagger_{\nu\sigma}(1-c^\dagger_{\nu\bar{\sigma}}c_{\nu\bar{\sigma}})+c^\dagger_{\nu\sigma}c^\dagger_{\nu\bar{\sigma}}c_{\nu\bar{\sigma}}$$
$$=c^\dagger_{\nu\sigma}(1-c^\dagger_{\nu\bar{\sigma}}c_{\nu\bar{\sigma}})+c^\dagger_{\nu\sigma}c^\dagger_{\nu\bar{\sigma}}(1-c^\dagger_{\nu\sigma}c_{\nu\sigma})c_{\nu\bar{\sigma}} .$$

We rewrite this relation as follows:

$$c^\dagger_{\nu\sigma}=a^\dagger_{\nu\sigma}+\sigma S^\dagger_\nu a^\dagger_{\nu\bar{\sigma}} \quad (\bar{\sigma}=-\sigma) , \tag{2.1a}$$

$$S^\dagger_\nu\equiv c^\dagger_{\nu+}c^\dagger_{\nu-} , \tag{2.1b}$$

$$a^\dagger_{\nu\sigma}\equiv c^\dagger_{\nu\sigma}(1-c^\dagger_{\nu\bar{\sigma}}c_{\nu\bar{\sigma}}) . \tag{2.1c}$$

The new operator $S^\dagger_\nu$ creates a nucleon pair and the other $a^\dagger_{\nu\sigma}$ creates an unpaired nucleon in a single-particle level ν.

From the definitions (2.1b) and (2.1c), we can obtain the commutation relations

$$[S_\nu,S^\dagger_\nu]=\delta_{\nu\nu'}(1-2N_\nu-v_\nu) , \tag{2.2a}$$

$$a_{\nu'\sigma'}a^\dagger_{\nu\sigma}+a^\dagger_{\nu\sigma}a_{\nu'\sigma'}=\delta_{\nu\nu'}\delta_{\sigma\sigma'}(1-a^\dagger_{\nu\bar{\sigma}}a_{\nu\bar{\sigma}})(1-N_\nu) , \tag{2.2b}$$

and the conditions

$$S^\dagger_\nu S^\dagger_\nu=a^\dagger_{\nu\sigma}a^\dagger_{\nu\sigma'}=a^\dagger_{\nu\sigma}S^\dagger_\nu=S^\dagger_\nu a^\dagger_{\nu\sigma}=a_{\nu\sigma}S^\dagger_\nu=0 , \tag{2.3}$$

where

$$N_\nu\equiv S^\dagger_\nu S_\nu , \tag{2.4a}$$

$$v_\nu\equiv a^\dagger_{\nu+}a^\dagger_{\nu+}+a^\dagger_{\nu-}a_{\nu-} . \tag{2.4b}$$

It is easy to show that N_ν and v_ν satisfy the relations

$$[N_\nu,S^\dagger_\nu]=S^\dagger_\nu,\ [N_\nu,a^\dagger_{\nu\sigma}]=0 ,$$
$$[v_\nu,a^\dagger_{\nu\sigma}]=a^\dagger_{\nu\sigma},\ [v_\nu,S^\dagger_\nu]=0 . \tag{2.5}$$

The relations (2.5) indicate that N_ν means the number of nucleon pairs $S^\dagger_\nu$ and v_ν means the number of unpaired nucleons $a^\dagger_{\nu\sigma}$ (i.e., the seniority number v_ν). The nucleon number in a level ν is given by $\sum_\sigma c^\dagger_{\nu\bar{\sigma}}c_{\nu\sigma}=2N_\nu+v_\nu$. The operators N_ν and v_ν have only the eigenvalue 0 or 1 because $N^2_\nu=N_\nu$ and $v^2_\nu=v_\nu$.

The above relations remind us of the "quantized" Bogoliubov-Valatin transformation in Refs. 10 and 11. That transformation, which is obtained in the spherical j-j coupling scheme, reduces to (2.1) in the case $j=\frac{1}{2}$. It should be noticed that $S^\dagger_\nu$ and $a^\dagger_{\nu\sigma}$ are simply expressed in terms of the original operator $c^\dagger_{\nu\sigma}$ and (2.1) is useful for both spherical and deformed nuclei.

Any operator can be expressed in terms of $S^\dagger_\nu$ and $a^\dagger_{\nu\sigma}$ through (2.1) and its matrix elements can be calculated from the operator rules (2.2)–(2.5). The pairing Hamiltonian is divided into two independent parts as follows:

$$H=\sum_{\nu\sigma}\epsilon_{\nu\sigma}c^\dagger_{\nu\sigma}c_{\nu\sigma}-\sum_{\mu\nu}G_{\mu\nu}c^\dagger_{\mu+}c^\dagger_{\mu-}c_{\nu-}c_{\nu+}$$
$$=H_S+H_a , \tag{2.6a}$$

$$H_s\equiv\sum_\nu 2\epsilon_\nu N_\nu-\sum_{\mu\nu}G_{\mu\nu}S^\dagger_\mu S_\nu , \tag{2.6b}$$

$$H_a\equiv\sum_\nu(\epsilon_{\nu+}a^\dagger_{\nu+}a_{\nu+}+\epsilon_{\nu-}a^\dagger_{\nu-}a_{\nu-}) , \tag{2.6c}$$

where

$$\epsilon_\nu\equiv(\epsilon_{\nu+}+\epsilon_{\nu-})/2 . \tag{2.7}$$

The first part, H_s, stands for the pairing degree of freedom and the second part, H_a, stands for the unpaired ones.

As H_s and H_a commute, the eigenstates of the pairing Hamiltonian are products of an eigenstate of H_s with one of H_a:

$$a^\dagger_{\nu_1\sigma_1}a^\dagger_{\nu_2\sigma_2}\cdots|2N\gamma[\nu_1\nu_2\cdots]\rangle , \tag{2.8a}$$

$$|2N\gamma[\nu_1\nu_2\cdots]\rangle$$
$$=\sum_{\mu_1\mu_2\cdots\mu_N\neq[\nu_1\nu_2\cdots]}f(\mu_1\mu_2\cdots\mu_N[\nu_1\nu_2\cdots])$$
$$\times S^\dagger_{\mu_1}S^\dagger_{\mu_2}\cdots S^\dagger_{\mu_N}|0\rangle . \tag{2.8b}$$

Here, N is the number of pairs $S^\dagger_\nu$, γ is the other quantum numbers, and $|0\rangle$ is the nucleon vacuum, i.e., $c_{\nu\sigma}|0\rangle=S_\nu|0\rangle=a_{\nu\sigma}|0\rangle=0$. The symbol [ ] means that the single-particle levels in it are blocked by unpaired nucleons $a^\dagger_{\nu\sigma}$.

B. Basic approximation for the pairing eigenstates

The states $|2N\gamma[\nu_1\nu_2\cdots]\rangle$ include the pairing vibrational excited states. In this paper, however, we concentrate our consideration on a special group of states which are composed of the lowest-energy state for each set of N and $[\nu_1\nu_2\cdots]$. We denote these states

$$|\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle . \tag{2.9}$$

The wave function (2.9) describes the configuration of N pairs with the largest energy gain when the single-particle levels $\nu_1\nu_2\cdots$ are excluded from the configuration space.

Let us define the projection operators

$$P_\nu\equiv 1-S^\dagger_\nu S_\nu,\ Q_\nu\equiv S^\dagger_\nu S_\nu , \tag{2.10}$$

where P_ν projects the states with the empty level ν and Q_ν projects the states with the filled level ν. These operators satisfy the following relations:

$$P_\nu+Q_\nu=1,\ P_\nu Q_\nu=0,\ P^2_\nu=P_\nu,\ Q^2_\nu=Q_\nu , \tag{2.11a}$$

$$S_\nu P_\nu=P_\nu S^\dagger_\nu=S^\dagger_\nu Q_\nu=Q_\nu S_\nu=0 , \tag{2.11b}$$

$$S^\dagger_\nu=S^\dagger_\nu P_\nu=Q_\nu S^\dagger_\nu , \tag{2.11c}$$

$$Q_\nu|\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle=0 \ \text{ for } \nu\in\nu_1\nu_2\cdots . \tag{2.11d}$$

Using P_ν and Q_ν, we can divide the wave function (2.9) into two parts, one having no nucleon in a certain level ν and the other having one pair of nucleons in that level ν:

$$|\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle=U_\nu(2N[\nu_1\nu_2\cdots])|P_\nu(2N[\nu_1\nu_2\cdots])\rangle+V_\nu(2N[\nu_1\nu_2\cdots])S^\dagger_\nu|Q_\nu(2N-2[\nu_1\nu_2\cdots])\rangle , \tag{2.12}$$

where

$$U_\nu(2N[\nu_1\nu_2\cdots])\equiv(\langle\langle\phi(2N[\nu_1\nu_2\cdots])\,|\,P_\nu\,|\,\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle)^{1/2}\,, \tag{2.13}$$

$$V_\nu(2N[\nu_1\nu_2\cdots])\equiv(\langle\langle\phi(2N[\nu_1\nu_2\cdots])\,|\,Q_\nu\,|\,\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle)^{1/2}\,,$$

and

$$|\,P_\nu(2N[\nu_1\nu_2\cdots])\rangle=P_\nu\,|\,\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle/U_\nu(2N[\nu_1\nu_2\cdots])\,, \tag{2.14a}$$

$$S_\nu^\dagger\,|\,Q_\nu(2N-2[\nu_1\nu_2\cdots])\rangle=Q_\nu\,|\,\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle/V_\nu(2N[\nu_1\nu_2\cdots])\,. \tag{2.14b}$$

The projected states (2.14a) and (2.14b) are normalized and orthogonal to each other. From the definition (2.13), V_ν^2 means the occupation probability of a nucleon pair in a level ν. Note that $U_\nu^2+V_\nu^2=1$. If there is no blocked level, (2.12) is the wave function of the ground state with nucleon number $2N$ ($|\,2N;\text{g.s.}\rangle$). Its schematic illustration is shown in Fig. 1. In the BCS approximation, because the number conservation is abandoned such as $|\,P_\nu(2N)\rangle\simeq|\,Q_\nu(2N-2)\rangle$, (2.12) is reduced to the usual BCS wave function.

It is complicated to describe the exact structures of the projected states $|\,P_\nu(2N[\nu_1\nu_2\cdots])\rangle$ and $|\,Q_\nu(2N-2[\nu_1\nu_2\cdots])\rangle$. However, since these projected states themselves are mixtures of a great number of configurations, they can be expected to resemble the lowest-energy states of the $2N$ and $2N-2$ nucleon systems with the blocked levels ν and $\nu_1\nu_2\cdots$:

$$|\,P_\nu(2N[\nu_1\nu_2\cdots])\rangle\simeq|\,\phi(2N[\nu\nu_1\nu_2\cdots])\rangle\rangle\,, \tag{2.15}$$

$$|\,Q_\nu(2N-2[\nu_1\nu_2\cdots])\rangle\simeq|\,\phi(2N-2[\nu\nu_1\nu_2\cdots])\rangle\rangle\,.$$

The approximation (2.15) is equivalent to writing Eq. (2.12) as follows:

$$|\,\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle\simeq U_\nu(2N[\nu_1\nu_2\cdots])\,|\,\phi(2N[\nu\nu_1\nu_2\cdots])\rangle\rangle+V_\nu(2N[\nu_1\nu_2\cdots])S_\nu^\dagger\,|\,\phi(2N-2[\nu\nu_1\nu_2\cdots])\rangle\rangle\,. \tag{2.16}$$

The idea of this approximation is similar to that of the BCS, but the nucleon number is conserved and the blocking effects are taken into account in our treatment.

The approximation (2.16) makes it possible to express various matrix elements in terms of the coefficients (U_ν,V_ν) as shown in Sec. III. The problem is how to get the coefficients (U_ν,V_ν). Various methods for determining (U_ν,V_ν) can be employed. We use the exact (U_ν,V_ν) obtained by the Richardson method[12,13] in the case of constant pairing force, as discussed in Sec. IV. In other cases of deformed nuclei there is no useful method for getting (U_ν,V_ν) better than the FBCS, because the shell model diagonalization and the Richardson method are not available. However, the simple way in Sec. III B related to the BCS equations including the blocking effects is useful in the superconducting phase. It is easy in spherical nuclei to get the exact (U_ν,V_ν) by the shell model diagonalization. Then our approach is also useful for spherical nuclei, although we do not pay attention to this in this paper.

III. EVALUATION OF VARIOUS MATRIX ELEMENTS

A. Examples of evaluation

As mentioned above, we suppose that the (U_ν,V_ν) have been already determined. This means also that the wave functions $|\,\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle$ and their energies $E(2N[\nu_1\nu_2\cdots])$ are known.

In order to show the way of evaluating other matrix elements under the approximation (2.16), we first consider the two-nucleon transfer matrix element between the ground states of adjacent even nuclei, which is calculated as

$$\begin{aligned}\langle 2N+2;\text{g.s.}\,|\,c_{\nu+}^\dagger c_{\nu-}^\dagger\,|\,2N;\text{g.s.}\rangle&=\langle\langle\phi(2N+2)\,|\,S_\nu^\dagger\,|\,\phi(2N)\rangle\rangle\\&\simeq\langle\langle\phi(2N[\nu])\,|\,V_\nu(2N+2)S_\nu S_\nu^\dagger U_\nu(2N)\,|\,\phi(2N[\nu])\rangle\rangle\\&=V_\nu(2N+2)U_\nu(2N)\,.\end{aligned} \tag{3.1}$$

This evaluation is very reasonable, while in the quasiparticle treatment there is an ambiguity as to whether the factors (U_ν,V_ν) appearing in (3.1) are derived from the $2N$ or $2N+2$ system.

The excited states with many unpaired nucleons are written, in our notation, as

$$|\,2N+l;\nu_1\sigma_1\cdots\nu_l\sigma_l\rangle=a_{\nu_1\sigma_1}^\dagger\cdots a_{\nu_l\sigma_l}^\dagger\,|\,\phi(2N[\nu_1\cdots\nu_l])\rangle\rangle\,. \tag{3.2}$$

Because no nucleon pair can occupy the blocked levels $\nu_1\cdots\nu_l$ in (3.2), the wave function of distributed pairs $|\,\phi(2N[\nu_1\cdots\nu_l])\rangle\rangle$ depends on the number of unpaired nucleons. Namely, the blocking effects can be taken into ac-

count in our treatment. The expectation value of the nucleon number in a level μ is obtained as follows:

$$\langle 2N+l;\nu_1\sigma_1\cdots\nu_l\sigma_l \mid \sum_\sigma c^\dagger_{\mu\sigma}c_{\mu\sigma} \mid 2N+l;\nu_1\sigma_1\cdots\nu_l\sigma_l\rangle = \begin{cases} 1 & \text{for } \mu\in\nu_1\cdots\nu_l\ , \\ 2(V_\mu(2N[\nu_1\cdots\nu_l]))^2 & \text{for } \mu\notin\nu_1\cdots\nu_l\ . \end{cases} \tag{3.3}$$

The energy of an excited state is given by

$$\langle 2N+l;\nu_1\sigma_1\cdots\nu_l\sigma_l \mid H \mid 2N+l;\nu_1\sigma_1\cdots\nu_l\sigma_l\rangle = E(2N[\nu_1\cdots\nu_l])+\epsilon_{\nu_1\sigma_1}\cdots+\epsilon_{\nu_l\sigma_l}\ , \tag{3.4a}$$

$$E(2N[\nu_1\cdots\nu_l]) = \langle\langle \phi(2N[\nu_1\cdots\nu_l]) \mid H \mid \phi(2N[\nu_1\cdots\nu_l])\rangle\rangle\ . \tag{3.4b}$$

Since the pairing eigenstates $\mid\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle$ do not include unpaired nucleons $a^\dagger_{\nu\sigma}$, the $\mid\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle$ are like vacuum states with respect to $a_{\nu\sigma}$:

$$a_{\nu\sigma}\mid\phi(2N[\nu_1\nu_2\cdots])\rangle\rangle = 0\ . \tag{3.5}$$

Therefore we can easily evaluate matrix elements between the states including unpaired nucleons by using the operation rules (2.2)—(2.5) and (3.5) in the same manner as (3.1).

For instance, the one-nucleon transfer matrix element between the state of the $2N+1$ system, $\mid 2N+1;\nu\sigma\rangle$, and the ground state of the $2N$ system, $\mid 2N;\text{g.s.}\rangle$, is calculated as

$$\begin{aligned}\langle 2N+1;\nu\sigma \mid c^\dagger_{\nu\sigma} \mid 2N;\text{g.s.}\rangle &= \langle\langle\phi(2N[\nu]) \mid a_{\nu\sigma}c^\dagger_{\nu\sigma}\mid\phi(2N)\rangle\rangle \\ &\simeq \langle\langle\phi(2N[\nu]) \mid a_{\nu\sigma}a^\dagger_{\nu\sigma}U_\nu(2N)\mid\phi(2N[\nu])\rangle\rangle \\ &= U_\nu(2N)\ .\end{aligned} \tag{3.6}$$

The last step follows by using the approximation (2.16) for $\mid\phi(2N)\rangle\rangle$. In our picture, the wave function of distributed pairs $\mid\phi(2N[\nu])\rangle\rangle$ in an odd-nucleon system is naturally different from $\mid\phi(2N)\rangle\rangle$ in an even-nucleon system, but the evaluation (3.6) is reasonable. Contrary to this, if one takes account of the blocking effects in the quasiparticle formalism, the calculation in (3.6) becomes confusing because the effects introduce different quasiparticle bases for the bra and ket vectors.[9]

B. Simple way of determining (U_ν, V_ν) in the superconducting state

Showing a rough evaluation of the energies $E(2N[\nu_1\nu_2\cdots])$, we give the simplest method for determining (U_ν,V_ν) in this subsection.

Although we suppose that the energies $E(2N[\nu_1\nu_2\cdots])$ are already known, the adoption of the approximation (2.16) makes it possible to express $E(2N[\nu_1\nu_2\cdots])$ in terms of (U_ν,V_ν) as follows:

$$\begin{aligned}E(2N[\nu_1\nu_2\cdots]) \simeq & \sum_{\nu(\neq\nu_1\nu_2\cdots)}(2\epsilon_\nu - G_{\nu\nu})(V_\nu(2N[\nu_1\nu_2\cdots]))^2 \\ & - \sum_{\mu\neq\nu(\neq\nu_1\nu_2\cdots)} G_{\mu\nu}V_\mu(2N[\nu_1\nu_2\cdots])V_\nu(2N[\nu_1\nu_2\cdots]) \\ & \times U_\mu(2N-2[\nu\nu_1\nu_2\cdots])U_\nu(2N-2[\mu\nu_1\nu_2\cdots])\ .\end{aligned} \tag{3.7}$$

This evaluation, of course, differs from the original one obtained in the process of determining (U_ν,V_ν). It should be noted here that the virtual contributions of pairing vibrational excitations to the interaction term $\sum_{\mu\nu}G_{\mu\nu}S^\dagger_\mu S_\nu$ are not included in (3.7). The evaluation (3.7) is also different from the BCS.

In a superconducting phase of many pairs distributed over many single-particle levels, the value of $U_\mu(2N-2[\nu\nu_1\nu_2\cdots])$ appearing in (3.7) is expected to be roughly equal to that of $U_\mu(2N[\nu_1\nu_2\cdots])$. If we make this approximation, (3.7) is reduced to the BCS energy, except that the blocking effects are included in it. In the case of constant pairing force $G_{\mu\nu}=G$, its variation equation gives

$$\begin{aligned}2\{\epsilon_\nu - G(V_\nu(2N[\nu_1\nu_2\cdots]))^2-\lambda\}U_\nu(2N[\nu_1\nu_2\cdots])V_\nu(2N[\nu_1\nu_2\cdots]) \\ = \{(U_\nu(2N[\nu_1\nu_2\cdots]))^2-(V_\nu(2N[\nu_1\nu_2\cdots]))^2\}\Delta\ ,\end{aligned} \tag{3.8a}$$

$$\Delta \equiv G\sum_{\nu(\neq\nu_1\nu_2\cdots)} U_\nu(2N[\nu_1\nu_2\cdots])V_\nu(2N[\nu_1\nu_2\cdots])\ , \tag{3.8b}$$

which are just the BCS equations including the blocking effects. Equations (3.8) are available for determining (U_ν, V_ν), if the BCS approximation is good. Once the BCS values of (U_ν, V_ν) have been obtained from (3.8), we can calculate a better energy than the BCS energy by substituting the BCS values of $V_\mu(2N[\nu_1\nu_2\cdots])$ and $U_\mu(2N-2[\nu\nu_1\nu_2\cdots])$ into (3.7). We can also evaluate other matrix elements by using the BCS values of (U_ν, V_ν) in the manner of Sec. III A. This simple but number-conserving method works better than the usual BCS.

The method in this subsection can be used as substitute for more precise one in the superconducting state. For weak pairing situations, however, it cannot be used, and then we must employ a more precise method, namely the Richardson method adopted in Sec. IV or the FBCS, in order to get (U_ν, V_ν).

IV. DISCUSSION

The preceding sections show that the present number-conserving formalism preserves an intimate correspondence to the quasiparticle approach. The matrix elements obtained have expressions similar to the BCS ones. Similar approaches starting with the FBCS wave functions were made by Lorazo and Quesne[2] and Li.[1] Lorazo and Quesne showed that the broken-pair model (FBCS) can take the place of the quasiparticle approach. Li's expressions of matrix elements obtained by an approximate number projection of the BCS wave function resemble our results. Both methods have the advantage that the coefficients (U_ν, V_ν) are consistently determined while in our method they are not. However, we need not confine the wave functions to the FBCS form. We can more correctly or exactly treat the pairing correlations in some weak pairing situations. Once the (U_ν, V_ν) have been determined, the evaluation of other matrix elements is very easy in our treatment.

The expression (3.1) of the two-nucleon transfer matrix element is the same as that obtained by Li.[1] According to Li's calculations in the Sn (spherical) nuclei, the approximation (3.1) can reproduce well the exact value. In deformed nuclei, although the exact calculation of this matrix element is difficult, the approximation (3.1) seems to be very good also. Our evaluation of two-body operators such as $\sum S_\mu^\dagger S_\nu$ in (3.7) is different from that of Li, because virtual contributions of pairing excitations are included in Li's result but not in ours. We can take account of the contributions in the same order approximation as Li, but we neglect them in this paper.

We now consider an example with a constant pairing force parameter $G_{\mu\nu}=G$, in which we can determine the occupation probabilities $(V_\nu(2N[\nu_1\nu_2\cdots]))^2$ and the energies $E(2N[\nu_1\nu_2\cdots])$ exactly by the Richardson method.[12,13] The Richardson method has not been used in realistic calculations because the evaluations of matrix elements are difficult and the numerical solution of its equations has not been established. As shown in the preceding sections, however, our basic approximation (2.16) makes it possible to evaluate matrix elements. We have also developed the numerical solution of the Richardson equations (see the Appendix). The calculations of V_ν^2 and E are not difficult compared with the FBCS calculations. We can thus use the Richardson method for finding exact energies and exact occupation probabilities. It works for any strength of G, even when the shell model calculation is practically impossible. Therefore, there is no reason to use other approximations for getting V_ν^2 and E in this constant pairing case.

Let us take a model which has 16 uniformly distributed levels with the parameters $\epsilon_{\nu\sigma}=\nu$ $(\nu=1,2,\ldots,16)$ and $G=0.5$ in arbitrary units. This model was used recently by Zeng *et al.*[14] to study the even-odd differences in the band-crossing frequency ω_c due to the blocking effects. A similar model was used in Ref. 15 before.

Table I shows the calculated occupation probabilities V_ν^2 and gap parameter Δ [Eq. (3.8b)] in the 16- and 17-nucleon systems. The exact result, which can be profitably used in our approach, is compared with the results of the truncated shell model made by Zeng *et al.*[14] and the BCS approximation including the blocking effects. The comparison with the exact result indicates that Zeng's calculation is insufficient. Contrary to their conclusion, the BCS approximation roughly reproduces the reduction of Δ in the odd nucleon system if the blocking effects are taken into account by using Eqs. (3.8). It should, however, be remembered that the inclusion of the blocking effects brings about confusion in calculations of matrix elements in the quasiparticle formalism.

Since exact calculations of other matrix elements, except for the energies and occupation probabilities, are difficult, it is impossible to check directly the accuracy of the evaluations of matrix elements shown in Sec. III A. To estimate the accuracy of the basic approximation (2.16), we calculate the energies of the ground state and the lowest excited states with the total seniority $v=2$ in the 16-nucleon system by using (3.7) derived through (2.16). The results are shown in Fig. 2. This figure confirms that the approximation (3.7) is better than the BCS one including the blocking effects [compare (A) and (B) with (C)]. The approximation (3.7) works well even if we use the (U_ν, V_ν) values calculated from the BCS equations (3.8) [compare (B) with (C)]. These results indirectly support the usefulness of the basic approximation (2.16). It is also worth mentioning that the simplified method in Sec. III B provides an improvement on the usual BCS.

Figure 2 still shows a discrepancy between (3.7) and the exact results. The errors partly come from neglecting the virtual contributions of pairing vibrational excitations as mentioned above. The effects do not exist in the matrix elements having only one $S_\nu^\dagger$ or S_ν, except for $(a_{\nu\sigma}^\dagger, a_{\nu\sigma})$. The above errors can be reduced considerably if we calculate the excitation energies measured from the ground-state energy with the aid of commutation relations. Of course, we need not adopt the approximation (3.7) in place of the exact energies.

For the [8,9] state in Fig. 2, the exact calculation gives the gap parameter $\Delta=1.037$, while the BCS equations including the blocking effects of the single-particle levels 8 and 9 provide only a trivial solution $\Delta=0$. For the [8,10] (or [7,9]) state, the exact Δ is 1.168, but the BCS one is merely 0.702. The BCS approximation is not good in

TABLE I. Comparison of the exact occupation probabilities V_ν^2 and gap parameter Δ with approximated ones. The state $|\phi(16[9])\rangle\rangle$ is the wave function of distributed pairs for the 17-nucleon system with a last odd nucleon in the level $\nu=9$. The exact results are obtained by the Richardson method. The configuration space in the shell model is truncated by limiting the configuration energy $E_c=\sum_\nu \epsilon_\nu$ to $E_c \leq 52$ as in Ref. 14. The self-energy correction for the single-particle energy of Eqs. (3.8) is not neglected in the BCS calculations.

	V_ν^2 in $\|\phi(16)\rangle\rangle$			V_ν^2 in $\|\phi(16)[9]\rangle\rangle$	
ϵ_ν	Exact	Shell	BCS	Exact	BCS
16	0.0218	0.0025	0.0168	0.0157	0.0083
15	0.0275	0.0048	0.0219	0.0199	0.0111
14	0.0358	0.0085	0.0295	0.0262	0.0155
13	0.0483	0.0144	0.0417	0.0358	0.0232
12	0.0685	0.0249	0.0627	0.0518	0.0381
11	0.1039	0.0446	0.1027	0.0813	0.0723
10	0.1724	0.0901	0.1868	0.1437	0.1732
9	0.3234	0.2246	0.3676		
8	0.6766	0.7754	0.6324	0.8607	0.8310
7	0.8276	0.9099	0.8132	0.9213	0.9290
6	0.8961	0.9554	0.8973	0.9499	0.9625
5	0.9315	0.9751	0.9373	0.9655	0.9771
4	0.9517	0.9856	0.9583	0.9748	0.9846
3	0.9642	0.9915	0.9705	0.9808	0.9890
2	0.9725	0.9952	0.9781	0.9849	0.9918
1	0.9782	0.9975	0.9832	0.9878	0.9936
Δ	2.113	1.396	2.062	1.499	1.333

these states because the pairing correlations are weak due to the blocking effects. These values of Δ in the lowest $v=2$ states are very different from $\Delta=2.113$ in the ground state. Accordingly, the usual quasiparticle approach with the same Δ can be improved. The present method is just powerful in such a case.

V. APPLICATION TO THE CRANKING MODEL

We conclude our consideration by giving a guide as to how the present method can be used.

We take up the cranked Hamiltonian

$$H_c=H-\omega J_x\ ,$$
$$J_x=\sum_{\nu\nu'}(j_x)_{\nu\nu'}\sum_\sigma \sigma c_{\nu\sigma}^\dagger c_{\nu'\sigma}\ . \tag{5.1}$$

The inclusion of the term $-\omega J_x$ in the HFB mean field brings about different quasiparticle bases for states with different angular velocities ω (or spin I). This feature is not appropriate for the description of band mixing, such as the backbending phenomena, because the calculation of matrix elements between the different states becomes difficult. This difficulty can be overcome by the configuration mixing treatment of the term $-\omega J_x$ on the quasiparticle basis fixed for $\omega=0$, or by working with constant an-

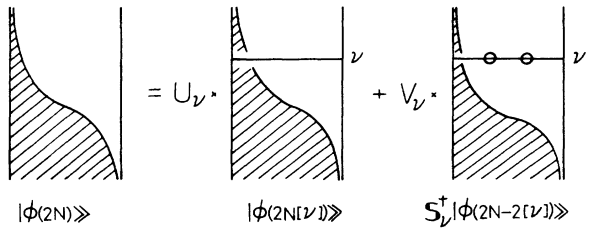

FIG. 1. Schematic illustration of the distribution of nucleon pairs expressed in (2.16).

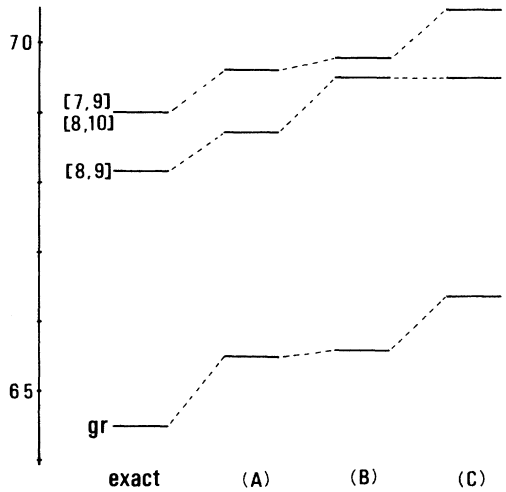

FIG. 2. Energies of the ground state and the lowest excited states with two unpaired nucleons in $[\mu,\nu]$, in the 16-nucleon system. The exact results are obtained by the Richardson method. The energies (A) and (B) are calculated through the approximation (3.7) by using the exact (U_ν,V_ν) values and the BCS ones, respectively. The results (C) show the usual BCS energies including the blocking effects.

gular momentum $\langle J_x \rangle$. The former seems to be good as long as ω is not too large. Then we can assume that H in (5.1) has the form (2.6) with $\epsilon_{\nu+}=\epsilon_{\nu-}=\epsilon_\nu$ and $G_{\mu\nu}=G$.

The configuration mixing treatment is very manageable by the present formalism. We can enjoy the advantage of the number-conserving treatment. The basis states corresponding to the many quasiparticle states are given by the eigenstates of H, which are written as

$$|\phi(2N)\rangle\rangle,\ a^\dagger_{\nu_1\sigma_1}a^\dagger_{\nu_2\sigma_2}|\phi(2N-2[\nu_1\nu_2])\rangle\rangle\ ,$$
$$a^\dagger_{\nu_1\sigma_1}a^\dagger_{\nu_2\sigma_2}a^\dagger_{\nu_3\sigma_3}a^\dagger_{\nu_4\sigma_4}|\phi(2N-4[\nu_1\nu_2\nu_3\nu_4])\rangle\rangle,\ \ldots\ . \tag{5.2}$$

We neglect the pairing vibrational excitations for the present. It should be noticed that the single-quasiparticle energies or routhians do not appear in our treatment of even nuclei. The energies of the basis states (5.2) are obtained exactly by the Richardson method as shown in Sec. IV. This is an important improvement on the usual quasiparticle treatment, because the number projection for the BCS formalism has the largest effect on the energies. The approximate evaluation of matrix elements presented in the preceding sections is applied to the term $-\omega J_x$. This approximation is not very bad because the term $-\omega J_x$ has only off-diagonal matrix elements between the basis states. Moreover, the present approximation is better than the BCS.

Through the transformation (2.1), J_x is written as

$$J_x=J_x^s+J_x^A\ , \tag{5.3a}$$
$$J_x^s\equiv\sum_{\nu\nu'}(j_x)_{\nu\nu'}\sum_\sigma\sigma(a^\dagger_{\nu\sigma}a_{\nu'\sigma}-S^\dagger_\nu a^\dagger_{\nu'\sigma}a_{\nu\sigma}S_{\nu'})\ , \tag{5.3b}$$
$$J_x^A\equiv\sum_{\nu\nu'}(j_x)_{\nu\nu'}\sum_\sigma(a^\dagger_{\nu\sigma}a^\dagger_{\nu'\bar\sigma}S_{\nu'}+S^\dagger_\nu a_{\nu\bar\sigma}a_{\nu'\sigma})\ . \tag{5.3c}$$

Here, J_x^s does not change the number of $a^\dagger$ (i.e., seniority number) and J_x^A changes it. Tanaka and Suekane[16] showed by the quasiparticle formalism that one can construct "the basic rotational bands" with different intrinsic properties by excluding J_x^A and the mixing of "the bands" can be treated by including J_x^A later. Their method is capable of describing the backbending phenomena without anomalies in the band crossing region.[17] More generally, however, we can diagonalize the term $-\omega J_x$ in a certain truncated space spanned by (5.2) under the constraint $\langle J_x\rangle=I$. The matrix elements of $-\omega J_x$ are easily evaluated by our method. Some of them are shown in the following:

$$\langle\langle\phi(2N-2[\nu_1\nu_2])|a_{\nu_2\sigma_2}a_{\nu_1\sigma_1}\omega J_x^s a^\dagger_{\nu_1'\sigma_1'}a^\dagger_{\nu_2'\sigma_2'}|\phi(2N-2[\nu_1'\nu_2'])\rangle\rangle$$
$$\simeq\delta_{\sigma_1\sigma_1'}\delta_{\nu_2\nu_2'}\delta_{\sigma_2\sigma_2'}\sigma_1\omega(j_x)_{\nu_1\nu_1'}$$
$$\times\{U_{\nu_1'}(2N-2[\nu_1\nu_2])U_{\nu_1}(2N-2[\nu_1'\nu_2'])-V_{\nu_1'}(2N-2[\nu_1\nu_2])V_{\nu_1}(2N-2[\nu_1'\nu_2'])\}$$
$$-(\nu_1\sigma_1\leftrightarrow\nu_2\sigma_2)-(\nu_1'\sigma_1'\leftrightarrow\nu_2'\sigma_2')+(\nu_1\sigma_1\leftrightarrow\nu_2\sigma_2\text{ and }\nu_1'\sigma_1'\leftrightarrow\nu_2'\sigma_2')\ , \tag{5.4a}$$

$$\langle\langle\phi(2N-2[\nu_1\nu_2])|a_{\nu_2\sigma_2}a_{\nu_1\sigma_1}\omega J_x^A|\phi(2N)\rangle\rangle\simeq\omega(j_x)_{\nu_1\nu_2}(U_{\nu_1}(2N-2[\nu_2])V_{\nu_2}(2N)-U_{\nu_2}(2N-2[\nu_1])V_{\nu_1}(2N))\ , \tag{5.4b}$$

where $(\nu_1\sigma_1\leftrightarrow\nu_2\sigma_2)$ in (5.4a) means exchanging $\nu_1\sigma_1$ for $\nu_2\sigma_2$ in the first term. The matrix elements (5.4b) are weakened by the factor $(U_{\nu_1}V_{\nu_2}-U_{\nu_2}V_{\nu_1})$. This is the well-known reason why the moment of inertia is reduced by the pairing correlations. From this reduction of J_x^A, we can expect that the mixings between the basis states with different seniorities become smaller.

Accordingly, we have a number-conserving treatment of the cranking model. The pairing correlations are quite accurately treated in our approach. In the calculated example of Sec. IV, Δ for the lowest basis states

$$a^\dagger_{\nu_1\sigma_1}a^\dagger_{\nu_2\sigma_2}|\phi(2N-2[\nu_1\nu_2])\rangle\rangle$$

is about a half of Δ for $|\phi(2N)\rangle\rangle$. This suggests that the blocking effects may have influence on the backbending point. The present treatment can properly take account of these effects, in contrast to the usual quasiparticle approach. It is also interesting to apply our method to the problem about the even-odd differences in the band-crossing frequency ω_c due to the blocking effects.[14,18]

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APPENDIX: SOLUTION OF THE RICHARDSON EQUATIONS

When $G_{\mu\nu}$ are constant ($G_{\mu\nu}=G$), the exact wave functions of the pairing states (2.8b) can be written as[12,13]

$$|2N\gamma[\nu_1\nu_2\cdots]\rangle=\prod_{k=1}^{N}\left[\sum_\nu{}'\frac{1}{2\epsilon_\nu-z_k}S_\nu^\dagger\right]|0\rangle\ , \tag{A1}$$

where z_k are roots of the coupled equations

$$\sum_\nu{}'\frac{1}{2\epsilon_\nu-z_k}=\frac{1}{G}+\sum_{k'(\neq k)}\frac{2}{z_{k'}-z_k}\quad(k=1,2,\ldots,N)\ . \tag{A2}$$

Here, $\sum_\nu'$ means the summation excluding the blocked levels $[\nu_1\nu_2\cdots]$. The exact energy and the exact expectation value of $N_\nu=S_\nu^\dagger S_\nu$ are given by

$$E(2N\gamma[\nu_1\nu_2\cdots])=\sum_{k=1}^{N}z_k\ , \tag{A3}$$

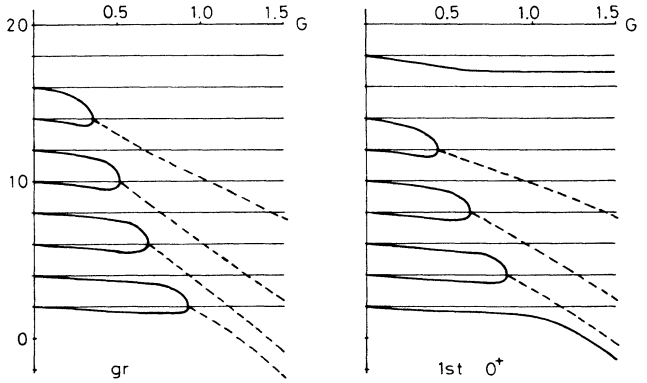

FIG. 3. The Richardson solutions in the schematic model adopted in Sec. IV ($\epsilon_\nu = 1,2,\ldots,16$): (a) the ground states and (b) the first excited 0^+ state, in the 16-nucleon system. The solid lines are the real roots and the dashed lines are the real parts of complex roots.

$$\{V_\nu(2N\gamma[\nu_1\nu_2\cdots])\}^2 = -G^2\frac{d}{dG}\sum_{k=1}^{N}\frac{1}{2\epsilon_\nu - z_k} . \quad \text{(A4)}$$

The Richardson equations (A2) have some complex conjugate roots $z_k = \xi_c \pm i\eta_c$ and the other real roots $z_k = z_r$ for a given value G. Equations (A2) are reduced to the following equations determining real quantities z_r, ξ_c, and η_c: A real root z_r satisfies the equations

$$\sum_\nu{}' \frac{1}{2\epsilon_\nu - z_r} = \frac{1}{G} + \sum_{r'(\neq r)}\frac{2}{z_{r'} - z_r} + \sum_c \frac{2(\xi_c - z_r)}{(\xi_c - z_r)^2 + \eta_c^2} , \quad \text{(A5a)}$$

and the real and imaginary parts of a pair of complex conjugate roots, (ξ_c, η_c), satisfy the equations

$$\sum_\nu{}' \frac{2\epsilon_\nu - \xi_c}{(2\epsilon_\nu - \xi_c)^2 + \eta_c^2} = \frac{1}{G} + \sum_r \frac{2(z_r - \xi_c)}{(z_r - \xi_c)^2 + \eta_c^2} + \sum_{c'(\neq c)} \frac{2(\xi_{c'} - \xi_c)}{(\xi_{c'} - \xi_c)^2 + (\eta_{c'} + \eta_c)^2} , \quad \text{(A5b)}$$

$$\sum_\nu{}' \frac{\eta_c^2}{(2\epsilon_\nu - \xi_c)^2 + \eta_c^2} = 1 + \sum_r \frac{2\eta_c^2}{(z_r - \xi_c)^2 + \eta_c^2} + \sum_{c'(\neq c)} \frac{2\eta_c(\eta_{c'} + \eta_c)}{(\xi_{c'} - \xi_c)^2 + (\eta_{c'} + \eta_c)^2} . \quad \text{(A5c)}$$

We show the numerical method by which to solve Eqs. (A5) in the model with uniformly distributed single-particle levels adopted in Sec. IV. The behaviors of the roots z_k are illustrated in Fig. 3. We can solve Eqs. (A5) by varying G from 0 to a given value step by step. In the case having no degenerate level, since all roots are real in a region of small G, we may solve only (A5a) by means of iteration in this region. As G increases, pairs of adjoining real roots become complex conjugate roots one after another. A pair of complex roots start when the left- and right-hand sides of (A5a) diverge (i.e., $z_k \to 2\epsilon_\nu$ and $z_{k+1} \to 2\epsilon_\nu$) and $(z_k + z_{k+1})/2$ crosses the horizontal line of $2\epsilon_\nu$. After the occurrence of complex roots, each set of ξ_c and η_c are determined from the crossing point of the two graphs (A5b) and (A5c). The consistent solutions of the entire coupled equations (A5) are obtained by means of iteration in each step when G increases.

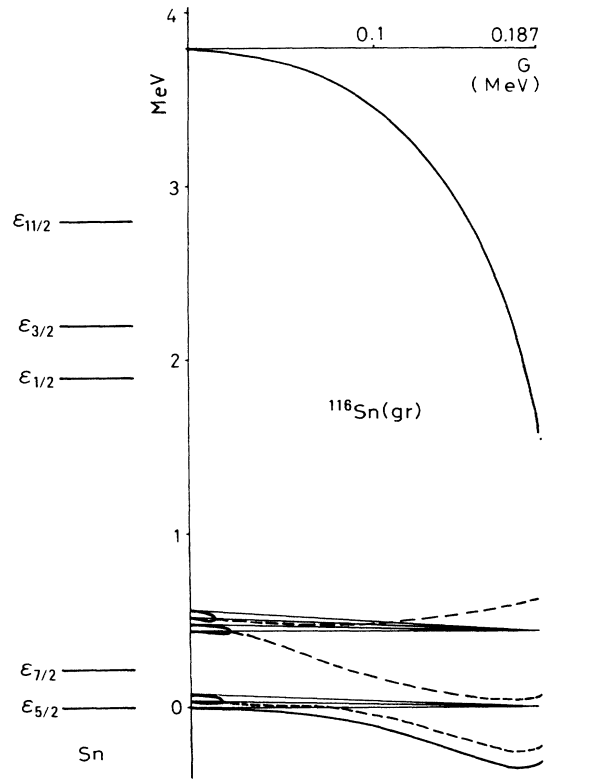

FIG. 4. The Richardson solution in the spherical nucleus ^{116}Sn, which has degenerate Nilsson levels. The single-particle parameters are the same as in Ref. 19. The levels $d_{5/2}$ and $g_{7/2}$ are forcibly split in the region of $G < 0.177$ MeV. The spacings between the split levels are 0.02 at $G = 0$ and zero at $G = 0.177$, in MeV.

The Richardson method is applicable to realistic cases in which the spacings of single-particle levels are arbitrary. To demonstrate this, we show the solution in the spherical nucleus ^{116}Sn, as a severe example which has many degenerate single-particle levels, in Fig. 4. In this figure the single-particle energies are varied with G so that the degenerate levels split in the region of $G < 0.177$. This technique makes it possible to solve any problems with degenerate levels. The results obtained in ^{116}Sn were confirmed to be correct by comparing them with the shell model results. It is worth noting that solving the Richardson equations is easier in deformed nuclei than in spherical nuclei.

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