Projection in the occupation-number space and the canonical transformation

1970 J. Phys. A: Gen. Phys. 3 8

(http://iopscience.iop.org/0022-3689/3/1/002)

Projection in the occupation-number space and the canonical transformation

V. N. FOMENKO

Physical Research Institute, Leningrad State University, Leningrad, U.S.S.R.

MS. received 4th June 1969

Abstract. In this paper a method for projecting the Bardeen–Cooper–Schrieffer states with respect to the particle number is suggested. This method does not involve the Fowler–Darwin integrals which are usually applied for this purpose. Energy matrix elements of an arbitrary single-particle operator and overlap integrals are calculated in the quasi-particle representation and are expressed analytically in terms of the u and v parameters. The volume of calculations according to the method suggested increases linearly with the size of the system in the case of factorizable pairing matrix elements (the weaker the particle-number fluctuations, the smaller the quantity of calculations). The method is illustrated by some model systems.

In the paper the limiting case of weak correlations is considered and comparison with perturbation theory is carried out.

1. Introduction

The Bardeen–Cooper–Schrieffer (1957, to be referred to as BCS) approach is applied widely in nuclear physics to the description of states when pairing forces are taken into consideration (Belyaev 1959). This method is especially successful in accounting for the two-quasi-particle states with seniority two and one-quasi-particle states (Kisslinger and Sorensen 1960, Pyatov and Soloviev 1964).

However, there is understandable disagreement with experiment which (as the calculations for several nuclei have shown (Richardson and Sherman 1964 a)) is accounted for, to a considerable extent, by the fact that the BCS trial wave function, borrowed from solid state theory, describes the nuclear states considerably more badly. It results from the smaller relative (i.e. divided by the constant of the pairing correlations) density of the levels of the average nuclear field. When applying the BCS approximation to the nuclear structure one should bear in mind that the BCS states are not the eigenstates of the particle-number operator. The number of particles that effectively take part in the correlations is not large because of the small density of the levels; the errors connected with non-conservation of the number of particles are appreciable. Kerman *et al.* (1961), using the projected (relative to the number of particles) BCS states, have shown that disagreement of the exact results and the BCS calculations may be accounted for practically only by the particle-number non-conservation.

In recent years a number of efforts have been made to solve the above-mentioned problem (Bayman 1960, Iwamoto and Onishi 1967, Chasman 1963, Richardson and Sherman 1964 b). Bayman considered the well-known integral of the Fowler–Darwin type, excluding fluctuations in the number of particles, by using the saddle-point approximation (i.e. for large fluctuations). However, this approach proved to be the usual BCS approximation. The corrections to the Bayman method were obtained by Iwamoto and Onishi using the approximation of large fluctuations. The methods of Chasman and of Richardson and Sherman employ the wave functions, strictly conserving the number of particles. However, these methods are rather complicated and do not allow generalizations in the cases of non-factorizable matrix elements. Fluctuations of the number of particles are excluded exactly in the paper by Dietrich *et al.* (1964) and the Fowler–Darwin integrals are calculated with the aid of the recurrence formulae. This method can also be used in

the case of the variable matrix elements of the pairing interaction. However, when we deal with real systems containing large numbers of particles, the quantity of calculation in this method increases rapidly. This is a defect of this method.

In this paper a new method free from the above-mentioned defects is suggested. In contrast with the other approaches this method does not use the integrals of the Fowler–Darwin type, though it includes the projecting procedure of the BCS states. The integrals are replaced by the sums; the number of terms in the sums is not large for real systems. In contrast with the methods using the saddle-point approximation the accuracy of projecting in our approach is higher (and not lower) for weak correlations if the quantity of calculations is the same. Thus, our method may be applied to the description of all the excited states with non-zero seniority.

As for the quantity of calculation, it increases practically linearly with the number of particles (for the factorizable matrix elements). Evidently, slower increase of the quantity of calculation (with increase of the system size) is impossible.

It should be noted that our method is a generalization of the representation suggested by Krutov for describing the excited paired states and considered in the paper by Krutov and Fomenko (1970). In this paper the states which are the particular case of the states considered in the present paper were used.

In § 2 we consider different variational approaches for solving the pairing Hamiltonian. In § 3 the method for projecting in occupation-number space is obtained. The matrix elements and overlap integrals are calculated in § 4 in the quasi-particle representation using the projected states. The limiting case of small correlations is investigated in § 5. Small correlations are shown to lead, in the variational approximation with particle-number conservation, to the trivial solution (no configuration mixing) only in the case when the pairing forces vanish. The comparison with perturbation theory is carried out. The results of the numerical calculations for some model systems illustrating the convergence of the method are presented in § 6.

2. Variational approach and particle-number conservation

The Hamiltonian of the pairing type for a system of neutrons or protons has the form (Belyaev 1959)

$$H = \sum_{\nu} (\epsilon_\nu - \lambda_f)(a_\nu^+ a_\nu + a_{-\nu}^+ a_{-\nu}) - \sum_{\nu'\nu} G_{\nu'\nu} a_{\nu'}^+ a_{-\nu'}^+ a_{-\nu} a_\nu. \tag{1}$$

In (1) a_ν^+ and a_ν are the particle creation and annihilation operators for the state $|\nu\rangle$, ϵ_ν is the single-particle energy of the average field, λ_f is the chemical potential, $G_{\nu'\nu}$ are the matrix elements of the pairing interaction, and the subscript ν labels the set of quantum numbers, $+\nu$ and $-\nu$ being related to each other by the time reversal.

Obviously, the Hamiltonian (1) has states which represent a system of particle pairs $a_\nu^+ a_{-\nu}^+|0\rangle$ scattered over average field levels and $|0\rangle$ is the particle-vacuum state. In this case we have the ground state or an excited one depending on the pair distribution over the levels.

States with unpaired particles $a_{\pm\nu}^+|0\rangle$ occupying some levels of the average field can also exist. Evidently these levels do not take part in pair scattering, the states of the other particles being determined only by the unblocked levels of the average field. These states can be described in the same way as the states without blocking.

In what follows we consider only states which can be reduced to the ground state with no levels blocked. This means that we do not consider the 0^+ excited states of the even proton or neutron system.

The state of the following form

$$|\psi\rangle = \prod_{\nu} (u_\nu + v_\nu a_\nu^+ a_{-\nu}^+)|0\rangle \tag{2}$$

is usually considered to describe approximately the system of paired particles.

This approximation is called the BCS approximation. The numbers u_ν and v_ν are hole and particle amplitudes, respectively. They satisfy the normalization condition $u_\nu^2+v_\nu^2=1$, or equivalently $v_\nu=\sin\varphi_\nu$, $u_\nu=\cos\varphi_\nu$. We shall assume in what follows with no loss of generality that $u_\nu \geqslant 0$.

In the BCS approximation the average number of particles in state (2) is made equal to the real number of particles in the system according to the following condition:

$$\langle\psi|\hat{N}|\psi\rangle = 2\sum_\nu v_\nu^2 = N \tag{3}$$

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

$$\hat{N} = \sum_\nu (a_\nu^+ a_\nu + a_{-\nu}^+ a_{-\nu}). \tag{4}$$

If one finds φ_ν by minimizing the form $\langle\psi|H|\psi\rangle$ and satisfying (3), one obtains (Belyaev 1959) the following expression for v_ν

$$v_\nu^2 = \tfrac{1}{2}\left[1-\frac{\bar{\epsilon}_\nu-\lambda_f}{\{(\bar{\epsilon}_\nu-\lambda_f)^2+\Delta_\nu^2\}^{1/2}}\right] \tag{5}$$

and the following system of superconductivity equations

$$2\Delta_{\nu'} = \sum_\nu G_{\nu'\nu}\frac{\Delta_\nu}{\{(\bar{\epsilon}_\nu-\lambda_f)^2+\Delta_\nu^2\}^{1/2}} \tag{6}$$

where $\bar{\epsilon}_\nu = \epsilon_\nu - G_{\nu\nu}v_\nu^2$ and the parameters λ_f and Δ_ν are derived from (3) and (6).

The wave function (2) is not an eigenstate of the Hamiltonian (1), whichever set of v_ν is used. It results from the fact that (2) is not an eigenstate of the particle-number operator unlike every eigenstate of the Hamiltonian (1). Thus (2) describes a superposition of states of several neighbouring nuclei (rather than a state of a given nucleus with a definite number of nucleons) with the same average field and with the number of nucleons differing by an even number.

Clearly, one obtains a more exact approximation when the component of (2) with the real number of particles is used as a trial function. This approximation was called the FBCS approximation (Dietrich *et al.* 1964, Mang *et al.* 1966). The approximation in which the state is described by the component of (2) with the correct number of particles with φ_ν the same as in the BCS approximation is also employed. Henceforth we shall denote this as the PBCS approximation (Kerman *et al.* 1961).

The BCS approximation can lead to noticeable errors; the PBCS approximation has been shown (by Kerman *et al.* 1961) to be in good agreement with the exact calculations for strong correlations. But the agreement becomes worse in the case of weaker correlations. The FBCS procedure is always good enough (Mang *et al.* 1966).

To make use of the PBCS or FBCS approximations one has to project out the proper component from (2), which in the following text will be called the physical component. In other words, one has to project states (2) in the occupation-number space.

The practical value of these approaches depends on the projection technique used.

If $|\phi\rangle$ is the projected BCS state (2), we can write

$$\langle\phi|H|\phi\rangle = \langle\psi|H|\psi\rangle + E(\varphi_\nu)$$

where $E(\varphi_\nu)$ is the correction to the BCS energy $\langle\psi|H|\psi\rangle$ due to the particle-number non-conservation. In this case the variational equations of the FBCS approximation can be written as follows:

$$\frac{\partial\langle\psi|H|\psi\rangle}{\partial\varphi_\nu}+\frac{\partial E(\varphi_\nu)}{\partial\varphi_\nu}=0. \tag{7}$$

Equation (7) should be solved by the iteration procedure. First, one solves the BCS equation

$$\frac{\partial \langle\psi|H|\psi\rangle}{\partial \varphi_\nu} = 0.$$

Then substituting the obtained $\varphi_\nu^{(0)}$ into $\partial E/\partial \varphi_\nu$ one solves the BCS-type equation but with the right-hand side

$$\frac{\partial \langle\psi|H|\psi\rangle}{\partial \varphi_\nu} = -\frac{\partial E(\varphi_\nu^{(0)})}{\partial \varphi_\nu}.$$

The $\varphi_\nu^{(1)}$ obtained from this equation are employed for calculating $\partial E/\partial \varphi_\nu$ and so on until the iteration process has converged. Certainly, not only the BCS solutions can be used as the first approximation for iteration.

The representation in the form of the integral of the Fowler–Darwin type is, as a rule, used for projection, the projected state with P particle pairs having the form

$$|\phi\rangle = (2\pi)^{-1/2} \frac{\oint (\mathrm{d}z/z^{P+1}) \prod_\nu (u_\nu + z v_\nu a_\nu^+ a_{-\nu}^+)|0\rangle}{\{\oint (\mathrm{d}z/z^{P+1}) \prod_\nu (u_\nu^2 + z v_\nu^2)\}^{1/2}} \tag{8}$$

where the integrals are calculated along the contour surrounding the $z = 0$ point.

Further, the matrix elements are calculated using $|\phi\rangle$. They are expressed in terms of integrals similar to the integrals in (8). The integrals obtained are calculated exactly (Dietrich *et al.* 1964) or in the saddle-point approximation (Bayman 1960, Iwamoto and Onishi 1967).

However, both methods have defects decreasing their practical value. The first method when applied to real systems is associated with too large a quantity of calculation. The second one can only be used in the case of strong particle-number fluctuations.

3. Formulation of the method

In the present paper we have chosen another way to project the BCS states (2) where no use is made of the integral representation (8).

We note that the state

$$\alpha^{-P} \prod_\nu (u_\nu + \alpha v_\nu a_\nu^+ a_{-\nu}^+)|0\rangle \tag{9}$$

(where α is a complex number not equal to zero) does not differ from the state (2) by its physical components since these components contain v_ν^P and α cancels. Hence the degree of freedom related to the choice of α is not physical. We shall use it to extract the physical components.

Let us consider the state

$$c\left\{\prod_\nu (u_\nu + v_\nu a_\nu^+ a_{-\nu}^+) + (-)^P \prod_\nu (u_\nu - v_\nu a_\nu^+ a_{-\nu}^+)\right\}|0\rangle \tag{10}$$

where c is the normalization constant.

One can easily see that the physical component in (10) is the same as in (2). However, the non-physical components in (2) with the number of pairs $P\pm1$, $P\pm3$, $P\pm5$,... are excluded from (10).

Let us consider the state

$$c\left[\prod_{\nu}(u_\nu+v_\nu a_\nu{}^+ a_{-\nu}{}^+)+(-)^P\prod_{\nu}(u_\nu-v_\nu a_\nu{}^+ a_{-\nu}{}^+)\right.$$
$$\left.+\mathrm{i}^{-P}\left\{\prod_{\nu}(u_\nu+\mathrm{i}v_\nu a_\nu{}^+ a_{-\nu}{}^+)+(-)^P\prod_{\nu}(u_\nu-\mathrm{i}v_\nu a_\nu{}^+ a_{-\nu}{}^+)\right\}\right]|0\rangle. \qquad (11)$$

Here, in addition, the components with the number of pairs $P\pm2$, $P\pm6$, $P\pm10$,... will be excluded because these components have equal values and opposite signs in the first and second lines of formula (11).

Using this procedure we can exclude all non-physical components. It can be formally proved as follows. Let us consider the state

$$|\tilde{\psi}_n\rangle = c\left[\prod_{\nu}(u_\nu+v_\nu a_\nu{}^+ a_{-\nu}{}^+)+(-)^P\prod_{\nu}(u_\nu-v_\nu a_\nu{}^+ a_{-\nu}{}^+)\right.$$
$$\left.+\left\{\sum_{k=1}^{n}\eta_k{}^{-P}\prod_{\nu}(u_\nu+\eta_k v_\nu a_\nu{}^+ a_{-\nu}{}^+)+\mathrm{c.c.}\right\}\right]|0\rangle \qquad (12)$$

where $\eta_k = \exp(\mathrm{i}\varphi k)$, $\varphi = \pi/(n+1)$ and n is a non-negative integer.

The amplitude in (12), corresponding to Q particle pairs occupying the levels $\mu_1,\ldots,\mu_Q$, has the form

$$c\prod_{\nu}u_\nu\prod_{\mu=\mu_1}^{\mu_Q}\frac{v_\mu}{u_\mu}\sum_{k=0}^{2n+1}\exp\{\mathrm{i}\varphi k(Q-P)\}. \qquad (13)$$

But

$$\frac{1}{2(n+1)}\sum_{k=0}^{2n+1}\exp(\mathrm{i}\varphi kM)=\begin{cases}0 & \text{if } M\neq 2l(n+1)\\ 1 & \text{otherwise}\end{cases}$$

where l is an integer.

Therefore, only the components with the pair numbers $P\pm2l(n+1)$ differ from zero in (12). If $2(n+1) > \max(P, L-P)$ (L is the total pair degeneracy of the system), then (12) gives the projected state (8), i.e. we have $|\tilde{\psi}_n\rangle = |\phi\rangle$. Certainly there is no practical need to eliminate all non-physical components because their amplitudes decrease rapidly when removing from the real number of particles $2P$. Indeed, the root-mean-square width of the wave packet with respect to the particle number

$$\sigma = \{\langle\psi|(\hat{N}-2P)^2|\psi\rangle\}^{1/2} = 2\left(\sum_{\nu}u_\nu{}^2v_\nu{}^2\right)^{1/2} \qquad (14)$$

does not exceed 3 for real cases. We shall consider the question of the choice of the value of n justified in practice in § 6 (the choice of too large a value of n makes the calculations complicated and does not change the result essentially; when too small a value of n is chosen, there remains a considerable admixture of non-physical components). Here we shall confine ourselves to the following remarks. The root-mean-square fluctuation (14) in the excited unpaired states is always smaller than in the ground state since the presence of the blocking particles leads to a decrease in the level density. Moreover, the fluctuations can be suppressed for the nuclei with the filled subshells. However, such states involve less numerical calculations in the present method because of the possibility of a decrease in n when the wave packet becomes narrower with respect to the particle number. We observe the opposite situation in other methods using the saddle-point approach where states with small correlations cannot be described satisfactorily.

4. Calculation of matrix elements with projected states

To obtain the matrix elements with the state (12) we pass over to the quasi-particle representation by means of the Bogoliubov–Valatin canonical transformation

$$\begin{aligned} \alpha_\nu &= u_\nu a_\nu - v_\nu a_{-\nu}^+ \\ \alpha_{-\nu} &= u_\nu a_{-\nu} + v_\nu a_\nu^+ \end{aligned} \tag{15}$$

where $\alpha_{\pm\nu}^+$ and $\alpha_{\pm\nu}$ are the creation and annihilation operators for quasi-particles. State (2) is the quasi-particle vacuum in the following sense:

$$\alpha_\nu|\psi\rangle = \alpha_{-\nu}|\psi\rangle = 0 \tag{16}$$

for arbitrary ν.

When the operators $A_\nu = \alpha_{-\nu}\alpha_\nu$ for quasi-particle pairs are introduced, one easily obtains the following expression

$$\begin{aligned} \prod_\nu (u_\nu + \eta_k v_\nu a_\nu^+ a_{-\nu}^+)|0\rangle = \prod_\nu (u_\nu^2 + \eta_k v_\nu^2)\Big\{1 + (\eta_k - 1)\sum_\mu \frac{u_\mu v_\mu}{u_\mu^2 + \eta_k v_\mu^2} A_\mu^+ \\ + \frac{(\eta_k-1)^2}{2} \sum_{\nu\neq\mu} \frac{u_\nu v_\nu u_\mu v_\mu}{(u_\nu^2 + \eta_k v_\nu^2)(u_\mu^2 + \eta_k v_\mu^2)} A_\nu^+ A_\mu^+ + \ldots\Big\}|\psi\rangle \end{aligned} \tag{17}$$

The operators we are interested in can also be written in the quasi-particle representation. In particular, the Hamiltonian (1) takes the form

$$H - \lambda\hat{N} = H_{00} + H_{11} + H_{20} + H_{22} + H_{31} + H_{40} \tag{18}$$

when the transformation (15) is carried out. In (18) λ labels an arbitrary reference level for the average field energies ϵ_ν and is introduced only to preserve the conventional form. H_{ik} denotes the sum of the component containing i creation and k annihilation quasi-particle operators normally ordered and the Hermite conjugate expression. To save space we do not cite the operators H_{ik}. They may be found in Belyaev's (1959) paper.

For calculating the matrix elements of the Hamiltonian (18) we shall make use of the fact that H is the operator conserving the particle number and connecting the components only with the equal numbers of particles. Therefore we have

$$\langle\tilde{\psi}_n|H|\eta_k{}^P \prod_\nu (u_\nu + \eta_k v_\nu a_\nu^+ a_{-\nu}^+)|0\rangle = \langle\tilde{\psi}_n|H|\psi\rangle. \tag{19}$$

Hence we can replace the matrix element $\langle\tilde{\psi}_n|H|\tilde{\psi}_n\rangle$ by $2(n+1)c\langle\tilde{\psi}_n|H|\psi\rangle$. Only the components of (18) that do not contain annihilation quasi-particle operators contribute in accordance with (16) to the latter matrix element, namely H_{00} and the corresponding parts of H_{20} and H_{40}. Thus, only the vacuum, two- and four-quasi-particle components of the expansion (17) are of interest for us.

Let us give the final formula for the expectation value of energy

$$\langle\tilde{\psi}_n|H|\tilde{\psi}_n\rangle = H_{00} + 2(n+1)c\langle\tilde{\psi}_n|H_{20} + H_{40}|\psi\rangle = H_{00} + \tilde{H}_{20} + \tilde{H}_{40} \tag{20a}$$

$$H_{00} = 2\sum_\nu (\epsilon_\nu - \lambda)v_\nu^2 - \sum_\nu u_\nu v_\nu \Delta_\nu - \sum_\nu G_{\nu\nu} v_\nu^4 \tag{20b}$$

$$\begin{aligned} H_{20} = &-\left(2\sum_k \epsilon_k R_k \cos\psi_k\right)^{-1} \\ &\times \sum_k \epsilon_k R_k \sum_\nu \{2\cos\psi_k \sin^2 x_k \delta_\nu + \sin\psi_k \sin(2x_k)\} \\ &\times \gamma_\nu \rho_{\nu k}{}^{-2}\{\gamma_\nu(\bar{\epsilon}_\nu - \lambda) - \delta_\nu \Delta_\nu\} \end{aligned} \tag{20c}$$

$$H_{40} = -\left(4\sum_k \epsilon_k R_k \cos\psi_k\right)^{-1} \sum_k \epsilon_k R_k \sin^2 x_k$$
$$\times [\cos\psi_k \{\cos^2 x_k (S_{00k} - T_{0k}) - S_{11k} + \sin^2 x_k (S_{22k} + T_{2k})\}$$
$$-\sin\psi_k \sin(2x_k)\{S_{10k} - S_{12k} - T_{1k}\}] \qquad (20d)$$

where

$$\gamma_\nu = 2u_\nu v_\nu, \qquad \delta_\nu = u_\nu^2 - v_\nu^2, \qquad \gamma_\nu^2 + \delta_\nu^2 = 1,$$
$$\tilde{\epsilon}_\nu = \epsilon_\nu - G_{\nu\nu} v_\nu^2, \qquad \Delta_\nu = \tfrac{1}{2}\sum_\mu G_{\nu\mu}\gamma_\mu,$$
$$\sum_k \equiv \sum_{k=0}^{n+1}, \qquad x_k = \frac{\varphi k}{2}, \qquad \epsilon_k = \begin{cases} \frac{1}{2} & \text{if } k = 0,\ n+1 \\ 1 & \text{otherwise} \end{cases}$$
$$R_k = \prod_\nu \rho_{\nu k}, \qquad \psi_k = \sum_\nu \varphi_{\nu k} + (L - 2P)x_k, \qquad (21)$$
$$\rho_{\nu k} = (1 - \sin^2 x_k \gamma_\nu^2)^{1/2}, \qquad tg\varphi_{\nu k} = -\delta_\nu tg x_k, \qquad |\varphi_{\nu k}| \leqslant \frac{\pi}{2},$$

$$S_{mnk} = \sum_{\nu\mu} \frac{G_{\nu\mu}\gamma_\nu \delta_\nu^{\,m} \gamma_\mu \delta_\mu^{\,n}}{\rho_{\nu k}^2 \rho_{\mu k}^2}, \qquad T_{nk} = \sum_\nu \frac{G_{\nu\nu}\gamma_\nu^4 \delta_\nu^{\,n}}{\rho_{\nu k}^4}.$$

In the case of the factorizable pairing matrix elements we have

$$G_{\nu\mu} = g_\nu g_\mu$$

and the expression (20*d*) becomes simpler, since in this case one should calculate only two sums instead of five (S_{00}, S_{10}, S_{11}, S_{12}, S_{22}).

$$s_{0k} = \sum_\nu g_\nu \frac{\gamma_\nu}{\rho_{\nu k}^2}, \qquad s_{1k} = \sum_\nu g_\nu \frac{\gamma_\nu \delta_\nu}{\rho_{\nu k}^2}$$

and we have

$$S_{mnk} = s_{mk} s_{nk}$$
$$s_{2k} = \frac{1}{\sin^2 x_k}\left\{\sum_\nu g_\nu \gamma_\nu - \cos^2 x_k s_{0k}\right\}.$$

Let $\hat{B}$ be an arbitrary single-particle operator conserving the number of particles (for instance, the electromagnetic moment). Then, proceeding in the way outlined above, one can obtain the matrix elements of $\hat{B}$ with projected states. We give some of them here:

$$\langle\tilde{\psi}_n|\hat{B}|\tilde{\psi}_n\rangle = B^{00} - \left(\sum_\nu \epsilon_k R_k \cos\psi_k\right)^{-1} \sum_k \epsilon_k R_k$$
$$\times \sum_\nu \{2\cos\psi_k \sin^2 x_k \delta_\nu + \sin\psi_k \sin(2x_k)\} \frac{\gamma_\nu B_{\nu-\nu}^{\,20}}{\rho_{\nu k}^2} \qquad (22a)$$

$$\langle\tilde{\psi}_{n\nu}|a_\nu \hat{B} a_\mu^+|\tilde{\psi}_{n\mu}\rangle = \left(\frac{\sum_k \epsilon_k R_k^{\,\mu} \cos\psi_k^{\,\mu}}{\sum_k \epsilon_k R_k^{\,\nu} \cos\psi_k^{\,\nu}}\right)^{1/2} B_{\nu\mu}^{\,11} - \left(\sum_k \epsilon_k R_k^{\,\nu} \cos\psi_k^{\,\nu} \sum_k \epsilon_k R_k^{\,\mu} \cos\psi_k^{\,\mu}\right)^{-1/2}$$
$$\times \sum_k \epsilon_k R_k^{\,\mu} \{2\cos\psi_k^{\,\mu} \sin^2 x_k \delta_\nu + \sin\psi_k^{\,\mu} \sin(2x_k)\} \frac{\gamma_\nu}{\rho_{\nu k}^2} \bar{B}_{-\nu\mu}^{\,20} \qquad (22b)$$

where the following notations were introduced

$$\hat{B} = B^{00} + \sum_{\rho\sigma} (B_{\rho\sigma}{}^{11}\alpha_\rho{}^+\alpha_\sigma + B_{\rho\sigma}{}^{20}\alpha_\rho{}^+\alpha_\sigma{}^+ + \bar{B}_{\rho\sigma}{}^{20}\alpha_\sigma\alpha_\rho) \tag{23}$$

$a_\nu{}^+|\tilde{\psi}_{n\nu}\rangle$ describes the projected state and the unpaired particle occupies the level ν. The quantities $R_k{}^\nu$ and $\psi_k{}^\nu$ are defined for the system of paired particles, with level ν excluded, according to formulae (21).

In particular, we have for the particle-number operator for level ν

$$\hat{N}_\nu = a_\nu{}^+ a_\nu + a_{-\nu}{}^+ a_{-\nu} \tag{4'}$$

the following expressions:

$$B^{00} = 2v_\nu{}^2, \qquad B_{\rho\sigma}{}^{11} = \delta_{\rho\sigma}(\delta_{\rho\nu} + \delta_{\rho-\nu})\delta_\nu$$

$$B_{\rho\sigma}{}^{20} = \bar{B}_{\rho\sigma}{}^{20} = \delta_{\rho-\sigma}(\delta_{\rho\nu} - \delta_{\rho-\nu})\frac{\gamma_\nu}{2}. \tag{24}$$

The overlap integrals which are employed in the calculations of the spectroscopic factors for β decay, (α, p) reactions and other processes have the following form:

$$\langle\tilde{\psi}_{1n}|\tilde{\psi}_{2n}\rangle = \left(\sum_k \epsilon_k R_{1k}\cos\psi_{1k} \sum_k \epsilon_k R_{2k}\cos\psi_{2k}\right)^{-1/2} \sum_k \epsilon_k R_{12k}\cos\psi_{12k} \tag{25}$$

with

$$\begin{aligned} R_{12k} &= \prod_\nu \rho_{12\nu k}, \qquad \psi_{12k} = \sum_\nu \varphi_{12\nu k} + (L-2P)x_k \\ \rho_{12\nu k} &= \{(u_{\nu 1}u_{\nu 2} + v_{\nu 1}v_{\nu 2})^2 - \sin^2 x_k \gamma_{\nu 1}\gamma_{\nu 2}\}^{1/2} \\ tg\varphi_{12\nu k} &= -\frac{u_{\nu 1}u_{\nu 2} - v_{\nu 1}v_{\nu 2}}{u_{\nu 1}u_{\nu 2} + v_{\nu 1}v_{\nu 2}} tgx_k \\ |\varphi_{12\nu k}| &\leqslant \frac{\pi}{2}\left(\geqslant \frac{\pi}{2}\right) \qquad \text{if} \qquad u_{\nu 1}u_{\nu 2} + v_{\nu 1}v_{\nu 2} \geqslant 0\,(\leqslant 0). \end{aligned} \tag{26}$$

The other notations are obvious. In formulae (20)–(26) the parameter n determines the extent to which non-physical components are excluded from $|\tilde{\psi}_n\rangle$ in the sense stated above.

As is seen from formulae (20)–(26), in the case of the factorizable pairing matrix elements the number of calculations of the matrix elements and overlap integrals with the projected states $|\phi\rangle$ increases quadratically with the number of particles in the system. Indeed, n increases linearly as well as the number of calculations connected with each term in the sum over k. However, our numerical estimates show that we can restrict ourselves to a rather small n (with practically no decrease in accuracy) both for large and small systems. This is possible due to the fact that the width of the wave packet (14) is not changed significantly when the size of the system increases. Thus, in the present method the quantity of calculation depends linearly on the number of particles in the system. In other words, the same number of calculations are required for a large system as for two systems of half its size. The method by Dietrich *et al.* (1964) in which integrals of type (8) are calculated exactly is more sensitive to the size of the system, since we consider finite sums containing a small number of terms instead of integrals (8). In the limit of infinite values of n the sums over k in formulae (20)–(26) will turn into integrals of the type (8) but the result remains the same as for finite n's. Thus, the mathematical

apparatus of the integrals of the Fowler–Darwin type is directly adjusted for treating infinite systems. However, in practice it is sufficient to describe finite systems containing only nucleons effectively taking part in the correlations, i.e. nucleons near the Fermi surface.

5. The limiting case of weak correlations

Let us now consider the limiting case of weak configuration mixing.

It can be seen from formula (13), which gives the expansion of the projected BCS state over the amplitudes of different orders† for $Q = P$, that the configuration mixing due to the pairing is stronger (weaker), the larger (smaller) the ratio v_μ/u_μ above (below) the Fermi surface. Since above (below) the Fermi surface $v_\mu/u_\mu \leqslant 1 (\geqslant 1)$, we can conclude that the larger γ_μ (equation (21)), the stronger the configuration mixing. It follows from (14) that the strong (weak) correlations, i.e. the configuration mixing, correspond to the large (small) root-mean-square fluctuations in the particle number (14) in the BCS state (2).

We shall now assume γ_ν to be small. First we shall prove that the configuration mixing ($\gamma_\nu \neq 0$) is present in the FBCS (i.e. in the variational approach treating the projected states as trial functions) no matter how small the $G_{\nu\mu}$ are. The presence of correlations in the case of very small $G_{\nu\mu}$ is easily seen, for example, from perturbation theory. However, the possibility of describing the weak correlations using an approximate method is not obvious. Meanwhile this is an important question because the most excited states with seniority two of heavy nuclei (Pyatov and Soloviev 1964) lie just in that region where the BCS approximation becomes a poor tool for describing the correlations.

To investigate the limit of γ_ν small we shall first expand the energy expectation value $\langle\phi|H|\phi\rangle$ in the series over γ_ν up to the second order (it should be remarked that only even orders are non-vanishing). It follows from (13) that the non-physical components with the number of pairs $Q = P+M$ (P being the real number of pairs) make the contribution of the order γ_ν^{2M}. Therefore, there is no need to exclude the components with $M \geqslant 2$. In this case it is sufficient to put $n = 0$ in (12). We then obtain from (20)

$$\langle\phi|H|\phi\rangle = \langle\tilde{\psi}_0|H|\tilde{\psi}_0\rangle + 0(\gamma_\nu{}^4) = 2\sum_{\nu\leqslant f}\epsilon_\nu - \sum_{\nu\leqslant f} G_{\nu\nu} - \tfrac{1}{2}\sum_{\nu\leqslant f}\sum_{\mu>f} G_{\nu\mu}\gamma_\nu\gamma_\mu + 0(\gamma_\nu{}^4). \qquad (27)$$

In (27) $\Sigma_{\nu\leqslant f}(\Sigma_{\mu>f})$ denotes the summation over occupied (empty) levels when $G_{\nu\mu} = 0$. As is seen from (27), small γ_ν do not correspond to the energy minimum. We conclude, therefore, that the correlations are present in the FBCS unless all $G_{\nu\mu}$ are equal to zero.

Our argument is valid only for the systems in which each level is either completely occupied or empty when $G_{\nu\mu} = 0$. If there are partially filled levels (spherical nuclei with partially filled subshells) and one restricts oneself to the case of the constant-pairing matrix elements $G_{\nu\mu} = G$, then γ_f (corresponding to the states f of the partially filled level ϵ_f) will never be small, because the many-particle states corresponding to this level are always involved in the superposition with equal amplitudes (as in the case of one degenerate level).

Since in this case not all γ_ν are small, the root-mean-square fluctuation (14) cannot be assumed to be small as well. For this reason we shall consider infinitely large $n (n \to \infty)$ in the formulae (20), thus introducing integrals. Then we obtain

$$\langle\phi|H|\phi\rangle = 2\sum_{\nu\leqslant f}\epsilon_\nu - GP - GP_f(\Omega_f - P_f) - G\{P_f\sum_{\nu>f}\gamma_\nu + (\Omega_f - P_f)\sum_{\nu<f}\gamma_\nu\}. \qquad (28)$$

† We follow here the terminology used by Chasman (1964) and call the amplitude of a state in which n particle pairs are excited and located above the Fermi surface the amplitude of the nth order.

In (28) P_f and Ω_f are the number of pairs in the level f when $G = 0$ and its pair degeneracy, respectively.

As follows again from (28), $\gamma_\nu = 0$ does not represent a stationary point for finite G and consequently there exist correlations in the FBCS states.

Let us now discuss the case of small G†. In this case we expand the series up to the quantities of the order γ_ν^4 and do not consider the quantities of the order $G\gamma_\nu^4$ when there are no partially filled levels, and we take into account the quantities of the order γ_ν^2 and drop those of the order $G\gamma_\nu^2$ when a partially filled level is present.

When there is no partially filled level we obtain

$$\langle\phi|H|\phi\rangle = 2\sum_{\nu\leqslant f}\epsilon_\nu + \tfrac{1}{8}\left(\sum_{\nu\leqslant f}\gamma_\nu^2\sum_{\mu>f}\epsilon_\mu\gamma_\mu^2 - \sum_{\nu>f}\gamma_\nu^2\sum_{\mu\leqslant f}\epsilon_\mu\gamma_\mu^2 - GP - \frac{G}{2}\sum_{\nu\leqslant f}\gamma_\nu\sum_{\mu>f}\gamma_\mu\right) \tag{29}$$

considering $n = 1$, in accordance with (13). For the case when there is a partially filled level we have

$$\begin{aligned}\langle\phi|H|\phi\rangle = {} & 2\sum_{\nu\leqslant f}\epsilon_\nu + \frac{P_f}{2(\Omega_f - P_f + 1)}\sum_{\nu>f}|\epsilon_\nu-\epsilon_f|\gamma_\nu^2 + \frac{\Omega_f - P_f}{2(P_f+1)} \\ & \times\sum_{\nu<f}|\epsilon_\nu-\epsilon_f|\gamma_\nu^2 - GP - GP_f(\Omega_f - P_f) - G\left\{P_f\sum_{\nu>f}\gamma_\nu + (\Omega_f - P_f)\sum_{\nu<f}\gamma_\nu\right\}\end{aligned} \tag{30}$$

taking $n \to \infty$.

From (29) and (30) one can obtain γ_ν corresponding to the energy minimum. When a partially filled level is absent we have

$$A_{\mu\nu} = \frac{\gamma_\mu\gamma_\nu}{4} = \frac{G}{2}\frac{E_1+E_2}{(E_1+\epsilon_\nu)(E_2-\epsilon_\mu)} \tag{31}$$

where $A_{\mu\nu}$ is the amplitude for the excitation of a pair of particles from the state $|\mu\rangle$ to the state $|\nu\rangle$ with the ground-state amplitude assumed to be unity. E_1 and E_2 satisfy the following system of equations:

$$\begin{aligned}E_1 &= -\sum_{\nu\leqslant f}\frac{\epsilon_\nu}{(E_2-\epsilon_\nu)^2}\left\{\sum_{\nu\leqslant f}\frac{1}{(E_2-\epsilon_\nu)^2}\right\}^{-1} \\ E_2 &= \sum_{\nu>f}\frac{\epsilon_\nu}{(E_1+\epsilon_\nu)^2}\left\{\sum_{\nu>f}\frac{1}{(E_1+\epsilon_\nu)^2}\right\}^{-1}.\end{aligned} \tag{32}$$

When a partially filled level is present, one obtains for the amplitudes

$$\begin{aligned}A_{\mu f} &= \frac{\gamma_\mu}{2}\left(\frac{\Omega_f - P_f}{P_f+1}\right)^{1/2} = \frac{G\{(P_f+1)(\Omega_f-P_f)\}^{1/2}}{2|\epsilon_\mu-\epsilon_f|} \\ A_{f\nu} &= \frac{\gamma_\nu}{2}\left(\frac{P_f}{\Omega_f - P_f+1}\right)^{1/2} = \frac{G\{P_f(\Omega_f-P_f+1)\}^{1/2}}{2|\epsilon_\nu-\epsilon_f|}.\end{aligned} \tag{33}$$

In (33) $A_{\mu f}$ is the amplitude of the state in which there are P_f+1 pairs on the level ϵ_f and no pair in the state $|\mu\rangle$, $A_{f\nu}$ corresponds to P_f-1 pairs on the level ϵ_f and one pair in the state $|\nu\rangle$, the amplitude of the ground state being assumed to be unity. The distribution of the pairs over other levels is the same as in the ground state at $G = 0$.

† For the sake of simplicity, we assume further $G_{\nu\mu} = G$.

The amplitudes (31) and (33) are proportional to G. On the other hand, the amplitudes in the first order of perturbation theory are also proportional to G. Therefore it is interesting to compare the results obtained with the perturbation theory results.

It can easily be seen from (31) that the amplitude $A_{\mu\nu}$ does not generally coincide with the perturbation-theory amplitude. Indeed, we have from (31)

$$\frac{A_{\mu\rho}}{A_{\nu\rho}} = \frac{A_{\mu\sigma}}{A_{\nu\sigma}}. \tag{34}$$

However, for the amplitudes obtained from perturbation theory we have

$$\frac{A_{\mu\rho}}{A_{\nu\rho}} = \frac{\epsilon_\rho - \epsilon_\nu}{\epsilon_\rho - \epsilon_\mu} \neq \frac{\epsilon_\sigma - \epsilon_\nu}{\epsilon_\sigma - \epsilon_\mu} = \frac{A_{\mu\sigma}}{A_{\nu\sigma}} \tag{35}$$

when $\epsilon_\rho \neq \epsilon_\sigma$. The relation (34) is a consequence of the separability of the amplitudes (Chasman 1963, 1964) of the BCS states (13) where each amplitude of the first order may be presented in the form

$$A_{\mu\nu} = c' D_\mu^{-1} D_\nu \tag{36}$$

where

$$D_\nu = \frac{v_\nu}{u_\nu}$$

and c' is the normalization constant. The approximation (36) considers the individual pairs of particles to be scattered independently of the configuration of the other particles, the probability for the level occupation being proportional to D_ν^2. This picture is real for bosons which are scattered independently. However, fermions correlate according to the Pauli principle. Of course, the quantities D_ν effectively take into account these correlations just as the Hartree–Fock field effectively includes two-body forces. But the relation (36) cannot generally yield the correct amplitudes. In particular, this relation contradicts perturbation theory in the case of weak correlations as we have seen above.

When there is no partially filled level, but all filled or empty levels are degenerate when $G = 0$, the result (31) coincides with the perturbation theory amplitudes. In this case separability (equation (36)) is no longer an approximation since the amplitudes depend only on one level above or below the Fermi surface. Similarly, the results (36) and the perturbation theory results coincide when there is a partially filled level.

6. Numerical estimates of the convergence of the method

The numerical calculations are performed for three model systems: the Pawlikowski–Rybarska (1962) model and two systems investigated by Richardson (1966) with the parameters $P = 4$, $G = 0{\cdot}8$ and $P = 16$, $G = 0{\cdot}375$.

The Pawlikowski–Rybarska model is a system of five equally spaced two-fold degenerate levels which contain six fermions. The level spacing and pairing interaction strength are assumed to be unity. The Richardson models are systems with two-fold degenerate levels with the level spacing assumed to be unity (P is the number of pairs in the system). The purpose of the numerical estimates being the investigation of the convergence of the method (i.e. the determination of practically justified n in (12) and (20)–(26)), only the ground states have been considered; the convergence for the excited states is certainly more rapid.

Table 1. Ground-state energies

System \ n	0	1	2	3	7	PBCS
$P-R$	−0·27	−1·20	—	—	—	−1·20
$P=4$	−0·12	−1·38	−1·41	—	—	−1·41
$P=16$	−0·07	−1·62	−1·88	−1·89	−1·89	−1·89

In table 1 the ground-state energies for the corresponding model systems are given, the BCS energy (i.e. H_{00}) being the reference level. The level spacing is used as a unit of energy (for heavy deformed nuclei this unit is approximately equal to 400 kev).

Table 2. Average occupation-probability corrections

System \ n	0	1	2	3	7	PBCS
$P-R$	0·0149	0·0537	—	—	—	0·0537
$P=4$	0·0066	0·0387	0·0392	—	—	0·0392
$P=16$	0·0041	0·0335	0·0355	0·0355	0·0355	0·0355

In table 2 the following quantities are given:

$$\frac{1}{L}\sum_{\nu}\left|\frac{\langle\tilde{\psi}_n|\hat{N}_\nu|\tilde{\psi}_n\rangle}{2}-v_\nu^2\right|$$

i.e. the occupation-probability corrections (averaged over the levels) connected with the projection of states using different n†.

In tables 1 and 2 the repeated results (when one moves from left to right) are omitted. They correspond to $n>n_0$, n_0 being the minimal integer for which $2(n_0+1)>\max(P, L-P)$, i.e. for which the projection is performed exactly.

One sees from tables 1 and 2 that $n=2$ ensures practically exact values of energy and occupation probabilities both for large and small systems with realistic parameter sets. It is worth noting that n can be further decreased for the excited states, especially for the first excited states with seniority two.

The formulae (20)–(26) can be simplified still more. According to our estimates, the quantities $T_{n\kappa}$ in (20*d*) contribute not more than 2–3% of the total correction (that is 20–30 kev) when P is about 15. For small systems, however, these terms can give more than 10% of the total contribution (more than 50 kev).

The angle ψ_1 in (20) was found to be approximately equal to 4° for the Pawlikowski–Rybarska model. Putting $\psi_1=0$ in the formulae (20) one obtains an error of 1% (nearly 5 kev). The angles ψ_κ are exactly equal to zero for the systems with the levels $\bar{\varepsilon}_\nu$ symmetric with respect to the chemical potential. The approximation $\psi_\kappa=0$ will probably be good enough for the real systems also.

Bearing in mind the results obtained, we should like to hope that our method (owing to its simplicity and accuracy) will increase the practical value of the variational approach with the conservation of the particle number (FBCS) and will make possible its wider applications to spectroscopic calculations and investigation of nuclear structure when the pairing Hamiltonian is solved.

† For the system with $P=16$, $G=0{\cdot}375$ the corrections were averaged only over the six levels nearest to the Fermi surface.

Acknowledgments

The author considers it to be his pleasant debt to thank Dr. V. A. Krutov for his interest in this work and for a number of valuable remarks. The author is also very grateful to Mr. L. N. Savushkin for his kind help in translating this text from Russian into English.

References

BARDEEN, J., COOPER, L. N., and SCHRIEFFER, J. R., 1957, *Phys. Rev.*, **108,** 1175–204.
BAYMAN, B. F., 1960, *Nucl. Phys.*, **15,** 33–8.
BELYAEV, S. T., 1959, *Matt.-Fys. Medd.*, **31,** 5–55.
CHASMAN, R. R., 1963, *Phys. Rev.*, **132,** 343–5.
—— 1964, *Phys. Rev.*, **134,** B279–84.
DIETRICH, K., MANG, H. J., and PRADAL, J., 1964, *Phys. Rev.*, **135,** B22–34.
IWAMOTO, F., and ONISHI, H., 1967, *Prog. Theor. Phys.*, **37,** 682–91.
KERMAN, A. K., LAWSON, R. D., and MACFARLANE, M. H., 1961, *Phys. Rev.*, **124,** 162–7.
KISSLINGER, L. S., and SORENSEN, R. A., 1960, *Matt.-Fys. Medd.*, **32,** 5–82.
KRUTOV, V. A., and FOMENKO, V. N., 1970, *Bull. Leningrad Univ.* No. 4, in the press.
MANG, H. J., RASMUSSEN, J. O., and RHO, M., 1966, *Phys. Rev.*, **141,** 941–8.
PAWLIKOWSKI, A., and RYBARSKA, W., 1962, *Sov. Phys.-JETP*, **43,** 543–50.
PYATOV, N. I., and SOLOVIEV, V. G., 1964, *Bull. Acad. Sci. USSR Phys. Ser.*, **28,** 1617–30.
RICHARDSON, R. W., 1966, *Phys. Rev.*, **141,** 949–56.
RICHARDSON, R. W., and SHERMAN, N., 1964 a, *Nucl. Phys.*, **52,** 253–68.
—— 1964 b, *Nucl. Phys.*, **52,** 221–38.

J. PHYS. A: GEN. PHYS., 1970, VOL. 3. PRINTED IN GREAT BRITAIN