Exact results for the particle-number-projected BCS approach with isovector proton-neutron pairing

A. A. Raduta,[1,2] M. I. Krivoruchenko,[3,4] and Amand Faessler[5]
[1]*Institute of Physics and Nuclear Engineering, P.O. Box MG06, Bucharest 077125, Romania*
[2]*Academy of Romanian Scientists, 54 Splaiul Independentei, Bucharest 050094, Romania*
[3]*Institute for Theoretical and Experimental Physics, B. Cheremushkinskaya 25, 117218 Moscow, Russia*
[4]*Department of Nano-, Bio-, Information and Cognitive Technologies, Moscow Institute of Physics and Technology, 9 Institutskii per., 141700 Dolgoprudny, Russia*
[5]*Institut für Theoretische Physik der Universität Tübingen, D-72076 Tübingen, Germany*
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The mean values of a many-body Hamiltonian including a proton-neutron pairing term and matrix elements of one-, two-, and four-body operators within a basis of particle-number-projected BCS states are analytically expressed in terms of a single function $Q(N)$ depending on the number of particles, N. The function $Q(N)$ is calculated using a recursion in N in which the shells and the BCS angles are kept the same for any iteration step. An illustrative example is numerically considered in a restricted single-particle space. Some specific features of the standard BCS, the projection after variation approach, and the variation after projection formalism are pointed out.

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I. INTRODUCTION

Shortly after the theory of superconductivity [1,2] showed up it has been realized [3] that such a formalism might work also for nuclear systems, although the number of constituents is relatively small. Many applications have been performed with a single constant for the interaction strength of various paired states. All calculations were based on the supposition that the particle number is conserved only on average. Amazingly, the pairing force and the emerging seniority scheme had been introduced much earlier, by Racah [4]. A serious question arose: namely, to what extent do particle number fluctuations affect some physical observables? Attempting to answer such a question many authors used a projected-particle-number formalism. Two distinct calculations have been employed. Occupation probabilities are determined first variationally with a standard BCS wave function and then the components of a given number of nucleons are projected out. The resulting procedure is conventionally called the particle-number-projected BCS and as we said already the projection is performed after variation. The second set of calculations perform the variation after projection. Particle number projection had been first considered by Bayman [5]. There the averages of the Hamiltonian, including the mean field and pairing terms, and of the particle number operator are expressed as functions of some residuum integrals which were estimated by the saddle-point method. The saddle point approximately satisfies an equation which is similar to the particle number equation of the BCS formalism. Under these conditions the Euler-Lagrange equations obtained with a particle-number-projected variational state are identical to the standard BCS equations. The projection procedure was improved in Refs. [6,7]. The residuum integrals were calculated by the saddle-point method with the integral path chosen such that it crosses the saddle point on a line of steepest descent. Moreover, two-dimensional recursion formulas for the residuum integrals were provided. An extensive analysis of ordinary BCS, PBCS (projected BCS with projection after variation), and FBCS (variation after projection) is performed within a two-level pairing model [7].

Another feature which was considered referred to the centrifugal Coriolis antipairing effect. The Coriolis interaction tends to decrease the pairing strength and at a critical angular frequency the gap equation has only a trivial solution. In Refs. [8,10] it is found that crossing the critical point the rotational energy exhibits a discontinuity, which, in fact, is not confirmed by the FBCS calculations of Ref. [7]. Clearly the occupation probabilities emerging from a FBCS formalism are different from those associated with ordinary BCS theory, the difference being a function of the pairing interaction strength. The idea of particle number projection was extended to angular momentum. Indeed, the cranking model with a particle-number-projected wave function was considered [9] to investigate the back-bending phenomena. The simultaneous projection of particle number and angular momentum from a pairing-correlated many-body system has been considered in Ref. [11] for light nuclei. Many papers have been devoted to the issues mentioned above [12], focusing on explaining properties such as gap parameter, moment of inertia, spectroscopic factors, pairing versus nuclear deformation, and angular momentum.

The field of the pairing interaction has been very much developed in the last three decades and many new issues have been addressed. Thus the differences and resemblances of pairing correlations in finite systems and infinite nuclear matter were pointed out by several authors [13–16]. The phenomenological way of determining the pairing correlations in finite nuclei does not determine uniquely the pairing interaction for the whole nuclear chart.

Microscopic approaches start from a bare N-N interaction, and at the next stage medium polarization effects are included [17–19]. In Refs. [20,21] an effective density-dependent

pairing interaction which reproduces both the neutron-neutron (nn) scattering length at zero density and the neutron pairing gap in uniform matter was proposed. In order to fulfill the two conditions an isospin dependence of the proposed effective interaction was necessary. This interaction was used in a Hartree-Fock-Bogoliubov calculations for the semi-magic isotopes of Ca, Ni, Sn, and Pb, which explained the binding energy dependence on the neutron number, the two-neutron separation energy, and the odd-even mass staggering. It was shown that supplementing the pairing interaction with an isovector term one can construct a global effective pairing interaction which is applicable to nuclei over a wide range of the nuclear chart [22].

The spatial dependence of the pairing gap in ^{120}Sn was studied in Ref. [23] based on the bare v_{14} Argonne N-N interaction supplemented with some important polarization effects. The spatial dependence of the pairing gap is obtained by multiplying the abnormal density by the N-N interaction. The Fourier transform with respect to the relative coordinate yields the gap dependence on the center-of-mass coordinate and relative momentum. The resulting gap is surface peaked, reflecting the dominant attractive character of the pairing interaction. The effect is more pronounced for lower momenta. The exchange with spin modes leads to an attractive component acting predilectly inside the nucleus and seems to be dominant in neutron matter. Various measures for spatial correlations were considered: rms of a Cooper pair, the coherence length, the average distance between the paired nucleons, etc. The pairing gap for uniform matter obtained from a microscopic treatment based on the realistic N-N interaction was considered in Ref. [16].

In Ref. [24] it was proved that the BCS equations work also for strongly interacting fermion systems which actually realize the so-called BEC phase characterized by a small coherence length in the coordinate space [25]. A regularized model for the density-dependent contact interaction, which removes the divergences showing up in the interaction strength and the scattering length, was used to study the transition between the BCS and the Bose-Einstein condensate (BEC) phases in symmetric, asymmetric, and neutron matter, respectively. Also the BEC-BCS crossover phenomena in dilute nuclear matter with a medium polarization effect included were investigated. There is a hope that the local density approximation opens up the possibility of mapping from the pairing in uniform nuclear matter to that in finite nuclei [26]. A full picture of achievements in the field of the pairing interaction may be found in some recent review papers [27].

Cooper pairs of one proton and one neutron have also been investigated [28–33], although not as extensively. The results reported there demonstrate that the generalized Bogoliubov-Valatin (BV) transformation including pp, nn, and pn pairing is appropriate for treating the pairing correlations in a self-consistent way, in spite of some earlier pessimistic views on this issue [34,35]. The results reported in Ref. [36], showing the isoscalar neutron-proton two-quasiparticle nature of the high-spin states in the $N = Z$ isotope of ^{92}Pd, support the existence of the $T = 0$ proton-neutron pairing in this system. Note that in a generalized (BV) formalism the total number of nucleons, the isospin third component (T_3), and isospin (T) are not conserved. Therefore a simultaneous projection for all three quantum numbers is necessary. This type of projection has been considered by several authors both numerically and analytically [37,38]. The integrability of a pn pairing model was treated in Refs. [39,40] by different methods. Thus the pairing Hamiltonian introduced by Richardson and Sherman [41] was considered in the context of the quantum inverse scattering method. It is proved that the model is integrable by constructing explicitly the conserved commuting operators. The eigenvalues of these operators were determined in terms of the Bethe ansatz and finally an expression for energy eigenvalues was possible [39]. A different method is applied, in Ref. [40], to the same Richardson model which includes isospin-symmetry breaking terms.

It seems that the common mathematical content with the above pairing-correlated system provides a serious ground for considering the pairing effect for other systems. Pairing forces acting among the quarks in two-color QCD matter lead to color superconductivity [42,43], as also confirmed by simulations in lattice gauge theories [44]. Superconductivity of metallic nanoparticles is discussed in Refs. [45–47]. Due to its paramount importance it is worth simplifying the formalism applied to other degrees of freedom by following the successful path used for pairing of like nucleons.

In this context the present paper considers the isovector pn pairing interaction with the projected total number of particles. We aim at obtaining tractable equations for the residuum integrals and finally for the norms and matrix elements of projected states.

This study is organized as follows. In Sec. II we study the factorization procedure applied to the exponent of a linear combination of the su(2) algebra generators. The motivation for this investigation is the fact that the BCS function could be obtained by transforming the particle vacuum state with such an operator. This is shown in Sec. III. The particle-number-projected function is described in Sec. IV. Analytical results of the average values of various interaction terms are given in Sec. V. Numerical results for a pairing Hamiltonian considered in a restricted single-particle space are given in Sec. VI. The final conclusions are collected in Sec. VII.

II. FACTORIZATION OF THE ROTATION OPERATOR

In the theory of superconductivity bilinear forms of creation and annihilation operators of fermions satisfy the commutation relations for the generators of rotations. For this reason, we shall first derive some very useful, in the theory of superconductivity, algebraic relations for the rotation operators. Although some of them are well known we present them for the sake of completeness.

In quantum mechanics, the rotation of a wave function is given by a real angle θ and the real unit vector $\mathbf{n}$,

$$\Psi \rightarrow \Psi' = \exp(-i\theta \mathbf{n}\mathbf{J})\Psi, \tag{2.1}$$

where $\mathbf{J}$ are the generators of rotation, given in Cartesian coordinates. We are interested in various equivalent representations of the rotation operators. Concretely, we wish to establish a connection between the rotation parameters θ, $\mathbf{n}$ from Eq. (2.1)

and those denoted by α_μ and β_μ ($\mu = \pm, 0$), which define two independent factorized forms for the same rotation operator

$$\begin{aligned}\exp(-i\theta\mathbf{nJ}) &\equiv U \\ &= \exp(i\theta n_- J_+ - i\theta n_0 J_0 + i\theta n_+ J_-) \\ &= \exp(i\alpha_- J_+)\exp(-i\alpha_0 J_0)\exp(i\alpha_+ J_-) \\ &= \exp(i\beta_+ J_-)\exp(-i\beta_0 J_0)\exp(i\beta_- J_+). \end{aligned} \quad (2.2)$$

The indices show the components of coordinates in the cyclic basis:

$$\mathbf{nJ} = -n_- J_+ + n_0 J_0 - n_+ J_-, \quad (2.3)$$

where

$$\begin{aligned} J_+ &= \frac{-1}{\sqrt{2}}(J_1 + iJ_2), \\ J_- &= \frac{1}{\sqrt{2}}(J_1 - iJ_2), \\ J_0 &= J_3. \end{aligned} \quad (2.4)$$

Throughout the present paper we use notation consistent with that of Ref. [48]. The spherical components of the unit vector are

$$\begin{aligned} n_\pm &= \mp\frac{1}{\sqrt{2}}\sin(\Theta)\exp(\pm i\Phi), \\ n_0 &= \cos(\Theta), \end{aligned} \quad (2.5)$$

where Θ and Φ are the polar and azimuthal angles. The unit length of the vector $\mathbf{n}$ implies, in the cyclic basis,

$$-2n_- n_+ + n_0^2 = 1. \quad (2.6)$$

The decomposition (2.2) resembles the representation of rotation as a product of three rotations described by the Euler angles. The difference is that here all three rotation generators are involved, and they are non-Hermitian operators.

The relation among the parameters θ, $\mathbf{n}$, and α_μ can be found by taking the derivative over θ of the left and right sides in Eq. (2.2) and using the commutation relations for the rotation generators. The derivative over θ gives

$$\begin{aligned}&(in_- J_+ - in_0 J_0 + in_+ J_-)\exp(-i\theta\mathbf{nJ}) \\ &\quad = i\alpha'_- J_+ \exp(i\alpha_- J_+)\exp(-i\alpha_0 J_0)\exp(i\alpha_+ J_-) \\ &\qquad - i\alpha'_0 \exp(i\alpha_- J_+) J_0 \exp(-i\alpha_0 J_0)\exp(i\alpha_+ J_-) \\ &\qquad + i\alpha'_+ \exp(i\alpha_- J_+)\exp(-i\alpha_0 J_0) J_- \exp(i\alpha_+ J_-). \end{aligned}$$

Here the prime symbol stands for the derivative with respect to the variable θ. Using the commutation relations satisfied by the angular momentum components [48]

$$\begin{aligned}[J_+, J_-] &= -J_0, \\ [J_\pm, J_0] &= \mp J_\pm, \end{aligned} \quad (2.7)$$

one finds

$$\begin{aligned}\exp(i\alpha_- J_+) J_0 \exp(-i\alpha_- J_+) &= J_0 - i\alpha_- J_+, \\ \exp(-i\alpha_0 J_0) J_- \exp(i\alpha_0 J_0) &= J_- \exp(i\alpha_0), \\ \exp(i\alpha_- J_+) J_- \exp(-i\alpha_- J_+) &= J_- - i\alpha_- J_0 - \frac{\alpha_-^2}{2} J_+. \end{aligned} \quad (2.8)$$

One thus arrives at the equation

$$\begin{aligned}&in_- J_+ - in_0 J_0 + in_+ J_- \\ &\quad = i\alpha'_- J_+ - i\alpha'_0 (J_0 - i\alpha_- J_+) \\ &\qquad + i\alpha'_+ \exp(i\alpha_0)\left(J_- - i\alpha_- J_0 - \frac{\alpha_-^2}{2} J_+\right), \end{aligned} \quad (2.9)$$

which can be split into three equations

$$\begin{aligned} n_- &= \alpha'_- + in_0\alpha_- + \frac{n_+\alpha_-^2}{2}, \\ n_0 &= \alpha'_0 + in_+\alpha_-, \\ n_+ &= \alpha'_+ \exp(i\alpha_0). \end{aligned} \quad (2.10)$$

Using the boundary conditions

$$\alpha_-(0) = \alpha_0(0) = \alpha_+(0) = 0,$$

we obtain

$$\alpha_\pm(\theta) = \frac{n_\pm 2\tan(\theta/2)}{1 + in_0\tan(\theta/2)}, \quad (2.11)$$

$$\alpha_0(\theta) = -2i\ln[\cos(\theta/2) + in_0\sin(\theta/2)]. \quad (2.12)$$

The result for the functions $\alpha_\mu(\theta)$ depends only on the commutation relations of J_μ and therefore is the same for any representation of the su(2) algebra generated by the angular momentum operators. Let us make use of this remark. Consider the fundamental representation and replace the operators J_μ by the Pauli matrices divided by 2. Next, we expand the left and right sides of the expression (2.2) in the parameters θ and α_μ. The decomposition over $\alpha_\pm$ is necessarily truncated at terms linear in $\alpha_\pm$ due to the equation $J_\pm^2 = 0$ being valid for the spin-1/2 representation. Thus, one obtains a system of algebraic equations for $\alpha_\mu(\theta)$ whose solutions, as can easily be checked, are given by Eqs. (2.11) and (2.12). The algebraic method is fully equivalent to solving the system of ordinary differential equations (2.10).

We assumed, so far, that the rotation angle θ and the unit vector $\mathbf{n}$ are real quantities. However, in the above development the condition for the mentioned variables to be real was not explicitly used. Equations (2.11) and (2.12), therefore, can be analytically continued to complex values of the parameter θ; the vectors $\mathbf{n}$ could also be complex under the condition that their square is equal to unity, i.e., $\mathbf{n}^2 = -2n_+n_- + n_0^2 = 1$. Obviously, these are the most general conditions. Any operator that can be written as the exponential of a linear combination of generators of the rotation with complex coefficients can be represented using a complex parameter θ and a unit complex vector $\mathbf{n}$.

In calculating the state norms and the matrix elements of operators one needs to know another factorized form for the rotation operator where the factor operators show up in the reverse order compared with that given in the second line of Eq. (2.2). The reverse order is shown explicitly in the third line of Eq. (2.2). We thus are looking for the rotation parameters β_μ as functions of θ and $\mathbf{n}$.

In the derivation of Eqs. (2.11) and (2.12) we have used only commutation relations for the generators of rotations. The explicit form of $\beta_\mu(\theta)$ can be obtained by using the fact that under the replacement of $(J_+, J_-, J_0) \to (J_-, J_+, -J_0)$

the commutation relations (2.7) remain unchanged. From this we immediately find

$$\beta_{\pm}(\theta) = \frac{n_{\pm} 2\tan(\theta/2)}{1 - i n_0 \tan(\theta/2)}, \tag{2.13}$$

$$\beta_0(\theta) = 2i \ln[\cos(\theta/2) - i n_0 \sin(\theta/2)]. \tag{2.14}$$

If we are able to express β_μ through α_μ, then we can change the order of the exponents with different operators J_μ. These relations are, however, simple:

$$\beta_{\pm} = -\alpha^*_{\mp}, \tag{2.15}$$

$$\beta_0 = \alpha^*_0. \tag{2.16}$$

Equations (2.15) and (2.16) are necessary and sufficient for the operator U to be unitary. They are therefore valid for real θ and for real unit vectors $\mathbf{n}$, which is for pure rotation. These equations cannot be continued analytically to complex values of θ and $\mathbf{n}$, because they involve the operation of complex conjugation. In the case of complex rotations, one should return to Eqs. (2.11) and (2.12). We express the complex parameters θ and $\mathbf{n}$ through α_μ, and we substitute these expressions in formulas (2.13) and (2.14). Simple calculations give

$$\beta_{\pm} = \frac{\alpha_{\pm}\exp(i\alpha_0)}{1 + \frac{1}{2}\alpha_+\alpha_-\exp(i\alpha_0)}, \tag{2.17}$$

$$\beta_0 = \alpha_0 + 2i \ln\left[1 + \tfrac{1}{2}\alpha_+\alpha_-\exp(i\alpha_0)\right]. \tag{2.18}$$

These formulas establish the connection between arbitrary complex parameters α_μ and β_μ. The inverse relations have the form

$$\alpha_{\pm} = \frac{\beta_{\pm}\exp(-i\beta_0)}{1 + \frac{1}{2}\beta_+\beta_-\exp(-i\beta_0)}, \tag{2.19}$$

$$\alpha_0 = \beta_0 - 2i \ln\left[1 + \tfrac{1}{2}\beta_+\beta_-\exp(-i\beta_0)\right]. \tag{2.20}$$

The factorized expression of any rotation-like operator is known in the literature as the Baker-Cambell-Haussdorff formula. The general necessary conditions which make this factorization possible are discussed in Ref. [49].

Inverse relations allowing defactorization of the rotation look as follows:

$$\begin{aligned}
\cos(\theta/2) &= \cos(\alpha_0/2) + \frac{1}{4}\alpha_+\alpha_-\exp(i\alpha_0/2) \\
&= \cos(\beta_0/2) + \frac{1}{4}\beta_+\beta_-\exp(-i\beta_0/2), \\
n_{\pm}\sin(\theta/2) &= \frac{1}{2}\alpha_{\pm}\exp(i\alpha_0/2) \\
&= \frac{1}{2}\beta_{\pm}\exp(-i\beta_0/2), \\
n_0\sin(\theta/2) &= \sin(\alpha_0/2) + \frac{i}{4}\alpha_+\alpha_-\exp(i\alpha_0/2) \\
&= \sin(\beta_0/2) + \frac{i}{4}\beta_+\beta_-\exp(-i\beta_0/2).
\end{aligned} \tag{2.21}$$

III. BCS STATE

The BCS wave function can be written as a unitary transformation of the vacuum state. Such a form significantly simplifies the calculations and gives physical meaning to the algebraic transformations involved in the formalism.

In the analogy with Eq. (2.1) one can write

$$|BCS\rangle = e^{-iF}|0\rangle, \tag{3.1}$$

where

$$F = \frac{1}{\sqrt{2}}\sum_{\alpha}\left(z_\alpha \sum_m c^\dagger_{\alpha m} d^\dagger_{\alpha\tilde{m}} + z^*_\alpha \sum_m d_{\alpha\tilde{m}} c_{\alpha m}\right) \tag{3.2}$$

is a Hermitian operator while $|0\rangle$ denotes the bare vacuum state. Here, $c^\dagger_{\alpha m}$ and $d^\dagger_{\alpha m}$ are particle creation operators for protons and neutrons, respectively, and α is the index numbering shells. For example, in a spherical shell model α is the set of quantum numbers (njl), where n is the radial quantum number, j is the total angular momentum, and l is the orbital angular momentum. $\tilde{m}$ denotes the time reversal substate: $d^\dagger_{\alpha\tilde{m}} = (-)^{j-m} d^\dagger_{\alpha,-m}$. For like nucleons in Ref. [50] and for a generalized pn pairing interaction in Ref. [38], analogous, otherwise different, unitary transformations have been used.

The creation operator images through the transformation $\exp(-iF)$ define the quasiparticle creation operators:

$$\begin{aligned}
e^{-iF} c^\dagger_{\alpha m} e^{iF} &= \mathfrak{c}^\dagger_{\alpha m}, \\
e^{-iF} d^\dagger_{\alpha m} e^{iF} &= \mathfrak{d}^\dagger_{\alpha m}.
\end{aligned} \tag{3.3}$$

with

$$\begin{aligned}
\mathfrak{c}^\dagger_{\alpha m} &= \cos\left(\frac{|z_\alpha|}{\sqrt{2}}\right) c^\dagger_{\alpha m} - i\frac{z^*_\alpha}{|z_\alpha|}\sin\left(\frac{|z_\alpha|}{\sqrt{2}}\right) d_{\alpha\tilde{m}}, \\
\mathfrak{d}^\dagger_{\alpha m} &= \cos\left(\frac{|z_\alpha|}{\sqrt{2}}\right) d^\dagger_{\alpha m} - i\frac{z^*_\alpha}{|z_\alpha|}\sin\left(\frac{|z_\alpha|}{\sqrt{2}}\right) c_{\alpha\tilde{m}}.
\end{aligned} \tag{3.4}$$

We recognize here the BV transformation

$$\begin{aligned}
\mathfrak{c}^\dagger_{\alpha m} &= U^p_\alpha c^\dagger_{\alpha m} - V^p_\alpha d_{\alpha\tilde{m}}, \\
\mathfrak{d}^\dagger_{\alpha m} &= U^n_\alpha d^\dagger_{\alpha m} - V^n_\alpha c_{\alpha\tilde{m}}.
\end{aligned} \tag{3.5}$$

By using the polar representation of the complex variable z,

$$z_\alpha = \frac{1}{\sqrt{2}}\rho_\alpha e^{-i\psi_\alpha}, \tag{3.6}$$

the occupation and nonoccupation probability coefficients, V and U, respectively, are expressed as follows:

$$\begin{aligned}
U^\tau_\alpha &= \cos\left(\frac{\rho_\alpha}{2}\right), \\
V^\tau_\alpha &= e^{i(\psi_\alpha + \frac{\pi}{2})}\sin\left(\frac{\rho_\alpha}{2}\right), \quad \tau = p, n.
\end{aligned} \tag{3.7}$$

The complex variable z_α can be interpreted as the $\mu = -1$ component of a representative vector from the associated classical phase space. From Eq. (3.7) it comes out that the BV transformation coefficients satisfy the normalization

conditions:

$$U_\alpha^2 + |V_\alpha|^2 = 1, \tag{3.8}$$

which assure that the quasiparticle operators obey anticommutation relations specific to fermions. Since $U_\alpha^p = U_\alpha^n$ and $V_\alpha^p = V_\alpha^n$, in what follows we shall omit the isospin index for the BV transformation coefficients. Applying the operator $\exp(-iF)$ on the obvious equations $c_{\alpha m}|0\rangle = d_{\alpha m}|0\rangle = 0$ one obtains $\mathfrak{c}_{\alpha m}|BCS\rangle = \mathfrak{d}_{\alpha m}|BCS\rangle = 0$, which expresses the fact that the BCS state is a vacuum state for the quasiparticle operators.

Using the proton and neutron creation operators one could define the bilinear operators

$$J_{\alpha+} = -\frac{1}{\sqrt{2}}\sum_m c_{\alpha m}^\dagger d_{\alpha\tilde{m}}^\dagger, \tag{3.9}$$

$$J_{\alpha-} = -\frac{1}{\sqrt{2}}\sum_m c_{\alpha m} d_{\alpha\tilde{m}}, \tag{3.10}$$

$$J_{\alpha 0} = \frac{1}{2}\sum_m (c_{\alpha m}^\dagger c_{\alpha m} - d_{\alpha m} d_{\alpha m}^\dagger), \tag{3.11}$$

which satisfy the su(2) algebra commutation relations [cf. Eqs. (2.7)]

$$\begin{aligned}[J_{\alpha+}, J_{\beta-}] &= -\delta_{\alpha\beta} J_{\alpha 0},\\ [J_{\alpha\pm}, J_{\beta 0}] &= \mp\delta_{\alpha\beta} J_{\alpha\pm}.\end{aligned} \tag{3.12}$$

We conventionally call these operators quasispin operators. Indeed, if we replace the d operators by c the resulting algebra defines the proton seniority states. Moreover, replacing the c operators by d one obtains the neutron quasispin algebra which defines the neutron seniority scheme. Although there is a danger of mixing them up with the angular momentum operator we use the notation J for the quasispin algebra operators. Actually, the pn pairing operators and the total number of nucleons form a representation of the su(2) algebra which is different from that generated by angular momentum components. Due to Eq. (3.12), the transformation e^{-iF} acquires the significance of a quasirotation. Within this context the quasiparticle operators appear to be the result of a quasirotation applied to the creation and annihilation particle operators.

It is worth mentioning some useful properties: $J_{\alpha\pm}^\dagger = -J_{\alpha\mp}$, $J_{\alpha 0}$ is a Hermitian operator. Due to the Pauli principle both $J_{\alpha+}$ and $J_{\alpha-}$ are nilpotent:

$$(J_{\alpha-})^{2j_\alpha+2} = (J_{\alpha+})^{2j_\alpha+2} = 0.$$

Acting on the vacuum state, one has

$$\begin{aligned}J_{\alpha-}|0\rangle &= 0,\\ J_{\alpha 0}|0\rangle &= -\left(j_\alpha + \tfrac{1}{2}\right)|0\rangle.\end{aligned}$$

For a given α the eigenstates of the proton-neutron pairing Hamiltonian in the restricted single-particle space can be expressed in terms of the irreducible representations of the SU(2) group. These are the states $|J_\alpha, J_{\alpha 0}\rangle$ which are simultaneous eigenstates for the operators J_α^2 and $J_{\alpha 0}$. The interpretation of the quasispin is revealed from the following obvious equations:

$$\begin{aligned}J_{\alpha-}|J_\alpha, -J_\alpha\rangle &= 0,\\ J_{\alpha 0}|J_\alpha, J_{\alpha 0}\rangle &= J_{\alpha 0}|J_\alpha, J_{\alpha 0}\rangle\\ &= \left(\frac{N}{2} - \frac{1}{2}(2j_a+1)\right)|J_\alpha, J_{\alpha 0}\rangle,\\ J_{\alpha 0} &= \frac{N}{2} - \frac{1}{2}(2j_\alpha+1).\end{aligned} \tag{3.13}$$

Since the values for N range from 0 to $2(2j_\alpha+1)$, the minimum and maximum values of $J_{\alpha 0}$ are $-(2j_\alpha+1)/2$ and $(2j_\alpha+1)/2$, respectively. Consequently, the quasispin has the expression

$$J_\alpha = \tfrac{1}{2}(2j_\alpha+1). \tag{3.14}$$

Thus, the state with a minimum quasispin projection to the z axis is a kind of Hartree-Fock vacuum for the lowering quasispin operator. Also, the component z of quasispin is related to the state angular momentum and the total number of particles, N, distributed on the substates of the single shell, j_α, while the quasispin is given by the semidegeneracy of the given single-particle state.

The transformation e^{-iF} is very useful for calculating operator matrix elements either in the quasiparticle or in the particle representation. As an example, we find the matrix element of a unit operator between the states $\exp(i\beta_{\alpha-}J_{\alpha+})|0\rangle$ and $\langle 0|\exp(i\beta_{\alpha+}J_{\alpha-})$.

By means of Eqs. (2.19) and (2.20), we obtain

$$\begin{aligned}&\langle 0|\exp(i\beta_{\alpha+}J_{\alpha-})\exp(i\beta_{\alpha-}J_{\alpha+})|0\rangle\\ &= \langle 0|\exp(i\alpha_{\alpha-}J_{\alpha+})\exp(-i\alpha_{\alpha 0}J_{\alpha 0})\exp(i\alpha_{\alpha+}J_{\alpha-})|0\rangle\\ &= \langle 0|\exp(-i\alpha_{\alpha 0}J_{\alpha 0})|0\rangle = \langle 0|\exp\left[i\alpha_{\alpha 0}\left(j_\alpha+\tfrac{1}{2}\right)\right]|0\rangle\\ &= \left(1+\tfrac{1}{2}\beta_{\alpha+}\beta_{\alpha-}\right)^{2j_\alpha+1}.\end{aligned} \tag{3.15}$$

In the above case, the parameter $\beta_{\alpha 0}$ is equal to zero; we used Eq. (2.20) to express $\alpha_{\alpha 0}$ in terms of $\beta_{\alpha+}$and $\beta_{\alpha-}$.

Under the unitary transformation, the generators $J_{\mu\alpha}$ become

$$e^{-iF}J_{\alpha\mu}e^{iF} = \mathfrak{J}_{\alpha\mu},\ \mu = \pm, 0,$$

where

$$\begin{aligned}\mathfrak{J}_{\alpha+} &= -\frac{1}{\sqrt{2}}\sum_m \mathfrak{c}_{\alpha m}^\dagger \mathfrak{d}_{\alpha\tilde{m}}^\dagger,\\ \mathfrak{J}_{\alpha-} &= -\frac{1}{\sqrt{2}}\sum_m \mathfrak{c}_{\alpha m}\mathfrak{d}_{\alpha\tilde{m}},\\ \mathfrak{J}_{\alpha 0} &= \frac{1}{2}\sum_m (\mathfrak{c}_{\alpha m}^\dagger \mathfrak{c}_{\alpha m} - \mathfrak{d}_{\alpha m}\mathfrak{d}_{\alpha m}^\dagger).\end{aligned} \tag{3.16}$$

Under the action of a unitary BV transformation, the operator $\exp(-iF)$ maps onto itself, since

$$\begin{aligned}\mathfrak{F} &\equiv e^{-iF}Fe^{iF}\\ &= \frac{1}{\sqrt{2}}\sum_\alpha\left(z_\alpha\sum_m \mathfrak{c}_{\alpha m}^\dagger\mathfrak{d}_{\alpha\tilde{m}}^\dagger + z_\alpha^*\sum_m \mathfrak{d}_{\alpha\tilde{m}}\mathfrak{c}_{\alpha m}\right)\\ &= F.\end{aligned} \tag{3.17}$$

The reciprocal relation for Eq. (3.3) takes the form

$$c_{\alpha m}^\dagger = e^{i\mathfrak{F}}\mathfrak{c}_{\alpha m}^\dagger e^{-i\mathfrak{F}}, \quad d_{\alpha m}^\dagger = e^{i\mathfrak{F}}\mathfrak{d}_{\alpha m}^\dagger e^{-i\mathfrak{F}}, \tag{3.18}$$

or, explicitly,

$$c^{\dagger}_{\alpha m} = U_{\alpha}\mathfrak{c}^{\dagger}_{\alpha m} + V_{\alpha}\mathfrak{d}_{\alpha\tilde{m}}, \quad d^{\dagger}_{\alpha m} = U_{\alpha}\mathfrak{d}^{\dagger}_{\alpha m} + V_{\alpha}\mathfrak{c}_{\alpha\tilde{m}}. \quad (3.19)$$

IV. PARTICLE NUMBER PROJECTION

The projection operator to the state with a definite number of particles is given by

$$P_N = \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{i(\hat{N}-N)\varphi}. \quad (4.1)$$

One can check that the signature property of a projection operator is satisfied:

$$P_N P_N = P_N. \quad (4.2)$$

The particle number operator can be expressed in terms of the operators $J_{\alpha 0}$ as

$$\hat{N} = \sum_{\alpha} \hat{N}_{\alpha},$$

where

$$\hat{N}_{\alpha} = 2J_{\alpha 0} + 2j_{\alpha} + 1. \quad (4.3)$$

The operator P_N acting on the BCS wave function gives a state with a definite number of particles,

$$|BCS, N\rangle \equiv C_N P_N |BCS\rangle = C_N \int_0^{2\pi} \frac{d\varphi}{2\pi} e^{-iN\varphi} e^{-iF(\varphi)}|0\rangle, \quad (4.4)$$

where

$$F(\varphi) = -\sum_{\alpha}(z_{\alpha}e^{2i\varphi}J_{\alpha+} - z^{*}_{\alpha}e^{-2i\varphi}J_{\alpha-}) \quad (4.5)$$

and $F = F(0)$.

By using the representation (3.6), the operator $F(\varphi)$ can be written as a sum of scalar products of vectors $\rho_{\alpha}\mathbf{n}_{\alpha}$ and quasispin operators $\mathbf{J}_{\alpha}$:

$$F(\varphi) = -\sum_{\alpha} \rho_{\alpha}\left(n_{\alpha-}J_{\alpha+} + n_{\alpha+}J_{\alpha-}\right). \quad (4.6)$$

Here, $\mathbf{n}_{\alpha}$ are unit vectors defined by the cyclic coordinates

$$n_{\alpha\pm} = \mp\frac{1}{\sqrt{2}}\exp[\pm i(\psi_{\alpha} - 2\varphi)], \quad n_{\alpha 0} = 0. \quad (4.7)$$

Using Eq. (2.2), we obtain

$$\exp[-iF(\varphi)] = \exp\left[i\sum_{\alpha}\rho_{\alpha}\left(n_{\alpha-}J_{\alpha+} + n_{\alpha+}J_{\alpha-}\right)\right] = \exp\left(i\sum_{\alpha}\alpha_{\alpha-}J_{\alpha+}\right) \times \exp\left(-i\sum_{\alpha}\alpha_{\alpha 0}J_{\alpha 0}\right)\exp\left(i\sum_{\alpha}\alpha_{\alpha+}J_{\alpha-}\right),$$

where, according to Eqs. (2.11) and (2.12),

$$\alpha_{\alpha\pm} = n_{\alpha\pm}2\tan(\rho_{\alpha}/2), \quad \alpha_{\alpha 0} = -2i\ln[\cos(\rho_{\alpha}/2)]. \quad (4.8)$$

Acting with the operator $\exp[-iF(\varphi)]$, after factorizing it, on the vacuum state, we obtain

$$\exp[-iF(\varphi)]|0\rangle = \prod_{\alpha}[\cos^2(\rho_{\alpha}/2)]^{j_{\alpha}+1/2} \times \exp\left[i\sum_{\beta}n_{\beta-}2\tan(\rho_{\beta}/2)J_{\beta+}\right]|0\rangle.$$

Now, we are in a position to find the projected state with N nucleons:

$$|BCS, N\rangle = C_N\int_0^{2\pi}\frac{d\varphi}{2\pi}\exp(-iN\varphi)\prod_{\alpha}[\cos^2(\rho_{\alpha}/2)]^{j_{\alpha}+1/2}\exp\left\{i\sum_{\alpha}\exp[i(-\psi_{\alpha}+2\varphi)]\sqrt{2}\tan(\rho_{\alpha}/2)J_{\alpha+}\right\}|0\rangle$$
$$= C_N\prod_{\alpha}[\cos^2(\rho_{\alpha}/2)]^{j_{\alpha}+1/2}\int_C\frac{d\zeta}{2\pi i}\frac{1}{\zeta^{N+1}}\exp\left[i\zeta^2\sum_{\alpha}\exp(-i\psi_{\alpha})\sqrt{2}\tan(\rho_{\alpha}/2)J_{\alpha+}\right]|0\rangle$$
$$= C_N\prod_{\alpha}[\cos^2(\rho_{\alpha}/2)]^{j_{\alpha}+1/2}\frac{1}{(N/2)!}\left(i\sum_{\alpha}\exp(-i\psi_{\alpha})\sqrt{2}\tan(\rho_{\alpha}/2)J_{\alpha+}\right)^{N/2}|0\rangle.$$

The contour C encompasses the point $\zeta = 0$, and the integration is performed in the direction of increasing $\varphi = \arg\zeta$.

By the condition (4.2), the problem of finding the normalization constant reduces to calculating the overlap of unprojected and projected states:

$$\langle BCS, N|BCS, N\rangle = C_N\langle BCS|BCS, N\rangle = C_N^2\prod_{\alpha}[\cos^2(\rho_{\alpha}/2)]^{2j_{\alpha}+1}\int_C\frac{d\zeta}{2\pi i}\frac{1}{\zeta^{N+1}}\langle 0|\exp\left[i\sum_{\alpha}\exp(i\psi_{\alpha})\sqrt{2}\tan(\rho_{\alpha}/2)J_{\alpha-}\right] \times\exp\left[i\zeta^2\sum_{\alpha}\exp(-i\psi_{\alpha})\sqrt{2}\tan(\rho_{\alpha}/2)J_{\alpha+}\right]|0\rangle$$
$$= C_N^2\int_C\frac{d\zeta}{2\pi i}\frac{1}{\zeta^{N+1}}\prod_{\alpha}[\cos^2(\rho_{\alpha}/2) + \zeta^2\sin^2(\rho_{\alpha}/2)]^{2j_{\alpha}+1}. \quad (4.9)$$

From the above equation we obtain

$$C_N^{-2} = \int_C \frac{d\zeta}{2\pi i} \frac{1}{\zeta^{N+1}} \prod_\alpha [\cos^2(\rho_\alpha/2) + \zeta^2 \sin^2(\rho_\alpha/2)]^{2j_\alpha+1}. \tag{4.10}$$

In the derivation of the expression (4.9), we used Eqs. (2.19) and (2.20), which allow us to change the order of the factors of the unitary operator. Also, we had to calculate the average of the product of exponents of operators associated with individual shells. If the two involved shells are distinct, the exponents commute with each other and their average over the vacuum is unity. An average value different from unity occurs only when the two shells coincide. The average value splits thereby into the product of the average values for the individual shells.

Further simplification can be achieved by using a binomial formula and then evaluating the integrand residue in the point $\zeta = 0$. After applying the binomial formula for the sum of a large number of terms and then finding the residue of the integrand the problem becomes combinatorial in nature, which is not attractive from the computational point of view, because the number of options needed to be considered and the number of terms in the sum grow with N exponentially.

From the computational point of view, the possibility of reducing the problem to evaluation of a recursion looks more attractive. We introduce the function

$$Q(N) = C_N^{-2} \tag{4.11}$$

with C_N^{-2} defined above.

Integrating by parts, one finds

$$Q(N) = \sum_\beta \int_C \frac{d\zeta}{2\pi i} \frac{\mathcal{G}_\beta(\zeta)}{\zeta^{N+1}}, \tag{4.12}$$

where

$$\mathcal{G}_\beta(\zeta) = \frac{\Omega_\beta}{N} \frac{\zeta^2 \sin^2(\rho_\beta/2)}{\cos^2(\rho_\beta/2) + \zeta^2 \sin^2(\rho_\beta/2)} \times \prod_\alpha [\cos^2(\rho_\alpha/2) + \zeta^2 \sin^2(\rho_\alpha/2)]^{2j_\alpha+1}, \tag{4.13}$$

with $\Omega_\beta = 2(2j_\beta + 1)$. We expand further the expression in front of the product sign in powers of ζ^2. Each member of the series is a function of $Q(N')$ for some value of $N' < N$. The function $Q(N)$, therefore, is expressed as the sum of $Q(N')$ evaluated for a smaller number of particles. It only remains to fix the boundary value for $N = 0$. From the definition of $Q(N)$ one easily finds

$$Q(0) = \prod_\alpha [\cos^2(\rho_\alpha/2)]^{2j_\alpha+1}. \tag{4.14}$$

Note that for negative integer values of N, the function $Q(N)$ is equal to zero, as can be seen from the Cauchy theorem related to the contour integral. Also, $Q(N) = 0$ for $N = 1$ mod(2). We thus get a recursion

$$Q(N) = \sum_\beta Q^\beta(N), \tag{4.15}$$

$$Q^\beta(N) = \frac{\Omega_\beta}{N} \sum_{n=1}^{N/2} (-)^{n+1} \tan^{2n}(\rho_\beta/2) Q(N - 2n). \tag{4.16}$$

The number of operations to calculate $Q(N)$ grows with increasing N only quadratically. From the viewpoint of numerical calculation, estimates for oscillatory contour integrals are associated with considerable difficulty. We avoid this difficulty by reducing the problem to the computation of the recursion relations. Within a variation after projection procedure the angles ρ_β are determined by the equations provided by the conditions that the energy of the system for a fixed N be minimum. The same angles are however used to calculate the factors $Q(N - 2n - 2)$ involved in the summation operation over n. The BCS angles as well as the number of involved shells are preserved during the iteration process.

The product factors from Eq. (4.13) can be expanded in a power series of $1/\zeta$. In this case we obtain a recursion for calculating the function $Q(N)$ starting from large numbers of particles. Recursion of this form is more convenient to calculate $Q(N)$ for values of N close to the maximum

$$\Omega = \sum_\beta \Omega_\beta. \tag{4.17}$$

Using the expansion in $1/\zeta$, we obtain Eq. (4.15) with

$$Q^\beta(N) = \frac{\Omega_\beta}{\Omega - N} \sum_{n=1}^{(\Omega-N)/2} (-)^{n+1} \cot^{2n}(\rho_\beta/2) Q(N + 2n). \tag{4.18}$$

These expressions should be supplemented by the boundary condition

$$Q(\Omega) = \prod_\alpha [\sin^2(\rho_\alpha/2)]^{2j_\alpha+1}. \tag{4.19}$$

For $N > \Omega$, the function $Q(N)$ is identically zero.

The only singularity of the integrand in the expression (4.12) is a pole at $\zeta = 0$. For this reason, we can deform the contour of integration, squeezing it around zero or moving it to infinity. In the first case, the expansion in powers of ζ is the appropriate one, while in the second case, the expansion in powers of $1/\zeta$ is valid. Obviously, the results (4.16) and (4.18) coincide. Also we note that for $N = 0$ the function $Q^\beta(N)$ given by Eq. (4.16) is not defined. For this case one should use the $1/\zeta$ expansion from Eq. (4.18). By contrast, for calculating $Q^\beta(\Omega)$ the expression (4.16) is the appropriate one. From the integral representation of $Q(N)$ as well as from Eq.(A11) considered for the diagonal case, a very simple relation follows:

$$\sum_{N=0}^{\Omega} Q(N) = 1. \tag{4.20}$$

By virtue of this expression, $Q(N)$ acquires the significance of the admixture probability of the N-projected state in the BCS wave function.

In realistic bases with a large number of shells, the recursion formulas (4.15) and (4.16) can lead to a numeric overflow because part of the shells remain almost empty and, therefore, have small BCS angles. In this case the function $Q(0)$ can

numerically vanish. To avoid this difficulty, we note that only the ratios of $Q(N)$ for different values of N matter, when matrix elements between projected states are calculated, while the overall normalization of $Q(N)$ is easily restored by Eq. (4.20). This means that at each step of the recursion, we could renormalize $Q(N)$ so that the maximum value in the sequence $Q(0), Q(2), \ldots, Q(N)$ is of the order of unity. Actually, the overall normalization is not important since all the matrix elements are expressed in terms of the ratios of $Q(N)$.

In the next section this will be shown for a few examples.

V. AVERAGE ENERGY

The projected state might be used as a variational state for a proton-neutron pairing Hamiltonian. We shall calculate the average of a many-body Hamiltonian with a two-body interaction with a strength depending on shells,

$$\hat{H} = \sum_{\alpha}(\epsilon_{\alpha} - \lambda)N_{\alpha} + \sum_{\alpha\beta}\mathcal{V}_{\alpha\beta}J_{\alpha+}J_{\beta-}. \tag{5.1}$$

Within the standard BCS formalism, λ is the Fermi sea level (chemical potential), which is to be fixed by solving the BCS equations. Here it is just a parameter involved in the gap energy equation. The two terms entering the microscopic Hamiltonian will be separately treated. The situation when $\mathcal{V}_{\alpha\beta} = 2G$ can be used to describe a possible transition of the pn system from the normal to the superconducting phase. Also such a Hamiltonian could be used for describing the rate of double-β Fermi-type decay. Note that such a particular form of the pn pairing interaction is not invariant under rotations in isospin space but preserves the third component, T_3, of the total isospin. Indeed, the two-body interaction comprises terms of isospin 0, 1, and 2. Therefore the eigenstates of $\hat{H}$ are expected to be a mixture of components of different isospin. In order to have an isospin-invariant Hamiltonian we have to account also for the pp and nn interaction. Due to these features we consider (5.1) as an illustrative example which allows us to describe the main ingredients of the present formalism.

A. Mean-field term

The mean-field energy is determined by averaging the particle number operator for each shell,

$$\langle N_{\alpha}\rangle = \langle BCS, N|N_{\alpha}|BCS, N\rangle. \tag{5.2}$$

With the interchange of the order of the exponent operators, as described in the previous section, this average is transformed into

$$\langle N_{\alpha}\rangle = Q^{-1}(N)\int_C \frac{d\zeta}{2\pi i}\frac{\mathcal{P}_{\alpha}(\zeta)}{\zeta^{N+1}}, \tag{5.3}$$

where

$$\mathcal{P}_{\alpha}(\zeta) = 2i\prod_{\gamma}[\cos^2(\rho_{\gamma}/2)]^{2j_{\gamma}+1}\frac{d}{dx}\langle 0|\exp\left[i\sum_{\gamma}\exp(i\psi_{\gamma})\right.$$
$$\left.\times\sqrt{2}\tan(\rho_{\gamma}/2)J_{\gamma-}\right]\exp\left[-ix\left(J_{\alpha 0}+j_{\alpha}+1/2\right)\right]$$
$$\times\exp\left[i\zeta^2\sum_{\gamma}\exp(-i\psi_{\gamma})\sqrt{2}\tan(\rho_{\gamma}/2)J_{\gamma+}\right]|0\rangle|_{x=0}. \tag{5.4}$$

The derivative over x is taken at $x = 0$. By making use of Eqs. (2.2), (2.19), and (2.20), $\mathcal{P}_{\alpha}(\zeta)$ can be simplified to give

$$\mathcal{P}_{\alpha}(\zeta) = N\mathcal{G}_{\alpha}(\zeta). \tag{5.5}$$

The function $\mathcal{G}_{\alpha}(\zeta)$ enters the definition of $Q(N)$ and is given by Eq. (4.13). Combining Eqs. (5.3) and (5.5), one obtains

$$\langle N_{\alpha}\rangle = NQ^{\alpha}(N)Q^{-1}(N). \tag{5.6}$$

The sum over α in Eq. (5.6) gives the identity $N = N$. Using Eq. (4.3), one can find the average of $J_{\alpha 0}$.

B. Energy gap function

Within the BCS theory the expression of the gap energy function is obtained by averaging the operator $\sqrt{2}\sum_{\alpha}J_{\alpha+}$ on the unprojected BCS state. Instead, for the particle-number-projected BCS formalism, the matrix element of the mentioned operator between the states with N and $N+2$ particles is to be calculated. We start by calculating such a matrix element for each term under summation:

$$\langle J_{\alpha+}\rangle = \langle BCS, N+2|J_{\alpha+}|BCS, N\rangle$$
$$= C_{N+2}\langle BCS|J_{\alpha+}|BCS, N\rangle. \tag{5.7}$$

The BCS wave functions of the initial and final states can be different ($\rho_{\alpha}\neq\rho'_{\alpha}$, $\psi_{\alpha}\neq\psi'_{\alpha}$). This case is considered in the Appendix. Here, following the path described in the previous section, we present results for the matrix elements diagonal in the BCS angles:

$$\langle J_{\alpha+}\rangle = -iQ^{-1/2}(N+2)Q^{-1/2}(N)\frac{1}{2\sqrt{2}}(N+2)$$
$$\times\exp(i\psi_{\alpha})\cot(\rho_{\alpha}/2)Q^{\alpha}(N+2). \tag{5.8}$$

Alternatively, one may express the above matrix elements as a polynomial in $\tan(\rho/2)$ by using a power expansion in ζ for the integrand, as explained already before. The result is

$$\langle J_{\alpha+}\rangle = iQ^{-1/2}(N+2)Q^{-1/2}(N)(2j_{\alpha}+1)\frac{1}{2\sqrt{2}}\exp(-i\psi_{\alpha})$$
$$\times\sum_{n=0}^{N}(-)^n\tan^{2n+1}(\rho_{\alpha}/2)Q(N-2n). \tag{5.9}$$

The matrix element of $J_{\alpha-}$ can easily be found by complex conjugation:

$$\langle J_{\alpha-}\rangle = \langle BCS, N|J_{\alpha-}|BCS, N+2\rangle$$
$$= -\langle J_{\alpha+}\rangle^*. \tag{5.10}$$

This quantity multiplied by $\sqrt{2}$ defines the spectroscopic factor for a pair α of states which could be measured in a deuteron transfer reaction. If the two-body interaction strength is state independent and equal to $2G$ the pairing interaction term resembles the pairing interaction for like nucleons. By virtue of particle number conservation, the average of $G\sqrt{2}\sum_{\alpha}J_{\alpha+}$

is equal to zero. By analogy with the case of like-nucleon pairing, we call the sum

$$\Delta_{pn}^{(N)} = G \sum_{\alpha} \langle BCS, N+2 | c_{\alpha m}^{\dagger} d_{\alpha \tilde{m}}^{\dagger} | BCS, N \rangle \quad (5.11)$$

the gap parameter for the N-nucleon system, which might be a good definition at least in the limit of large N.

C. Interaction energy

Now, consider the proton-neutron (pn) pairing interaction with the generic term:

$$\langle J_{\alpha+} J_{-\beta} \rangle = \langle BCS, N | J_{\alpha+} J_{\beta-} | BCS, N \rangle. \quad (5.12)$$

First, we lift the operators $J_{\alpha+}$ and $J_{\beta-}$ to the arguments of exponents by introducing two derivatives over x and y, evaluated at the origin:

$$\langle J_{\alpha+} J_{\beta-} \rangle = Q^{-1}(N) \int_C \frac{d\zeta}{2\pi i} \frac{\mathcal{P}_{\alpha\beta}(\zeta)}{\zeta^{N+1}},$$

where

$$\begin{aligned} \mathcal{P}_{\alpha\beta}(\zeta) = & -\prod_{\gamma} [\cos^2(\rho_\gamma/2)]^{2j_\gamma+1} \frac{d}{dx}\frac{d}{dy} \langle 0| \\ & \times \exp\left[i \sum_{\gamma} \exp(i\psi_\gamma) \sqrt{2} \tan(\rho_\gamma/2) J_{\gamma-} \right] \\ & \times \exp(-ixJ_{\alpha+}) \exp(-iyJ_{-\beta}) \\ & \times \exp\left[i\zeta^2 \sum_{\delta} \exp(-i\psi_\delta) \sqrt{2} \tan(\rho_\delta/2) J_{\delta+} \right] \\ & \times |0\rangle \,|_{x=y=0}. \end{aligned} \quad (5.13)$$

The product of four exponents is then reordered, using the results of Sec. II.

The final expressions for $\alpha \neq \beta$ and $\alpha = \beta$ become

$$\begin{aligned} \langle J_{\alpha+} J_{\beta-} \rangle = & \, Q^{-1}(N) \frac{1}{4} N[(2j_\beta+1)Q^{\alpha}(N) - (2j_\alpha+1)Q^{\beta}(N)] \\ & \times \frac{\exp(i\psi_\beta - i\psi_\alpha) \tan(\rho_\beta/2) \tan(\rho_\alpha/2)}{\tan^2(\rho_\beta/2) - \tan^2(\rho_\alpha/2)}, \end{aligned} \quad (5.14)$$

$$\begin{aligned} \langle J_{\alpha+} J_{\alpha-} \rangle = & -Q^{-1}(N) \left[\frac{N}{2} Q^{\alpha}(N) + (j_\alpha + 1/2) \sum_{n=1}^{N/2} (-)^{n+1} \right. \\ & \left. \times \tan^{2n}(\rho_\alpha/2)(2nj_\alpha - 1) Q(N-2n) \right]. \end{aligned} \quad (5.15)$$

In the standard BCS formalism, according to Eq. (3.6) the occupation probabilities for protons and for neutrons associated with the single-particle state $|\alpha\rangle$ are equal to each other:

$$\left| V_\alpha^p \right|^2 = \left| V_\alpha^n \right|^2. \quad (5.16)$$

Within a particle-number-projected formalism, the occupation probability is different from that defined above. Indeed, here the occupation probability for the pair of α states is given by

$$-2\langle J_{\alpha+} J_{\alpha-} \rangle \neq \sin^2(\rho_\alpha/2). \quad (5.17)$$

VI. ONE- AND TWO-SHELL CASES

In this section we shall focus on the pairing Hamiltonian

$$\begin{aligned} \hat{H} = & \sum_{\alpha m} (\epsilon_\alpha - \lambda)(c_{\alpha m}^{\dagger} c_{\alpha m} + d_{\alpha m}^{\dagger} d_{\alpha m}) \\ & - G \sum_{\alpha\beta mn} c_{\alpha m}^{\dagger} d_{\alpha \tilde{m}}^{\dagger} d_{\beta \tilde{n}} c_{\beta n}. \end{aligned} \quad (6.1)$$

In the special situation when the single-particle space occupied by protons and neutrons is restricted to a single j, the energy for N nucleons calculated as the average of $\hat{H}$ corresponding to $\lambda = 0$ with the N-projected state defined before is a quantity growing quadratically with N and depending neither on ρ nor on ψ. In this respect, one may say that the N-projected state does not exhibit a superconducting character. However, the spectroscopic factors defined by Eq. (5.10) can be calculated if ρ and ψ are determined within the standard BCS theory. In that case, the spectroscopic factor is readily obtained once the functions $Q(N)$ are calculated.

After some algebraic manipulations one finds a binomial distribution

$$Q(N) = \binom{2j+1}{N/2} p^{N/2} (1-p)^{2j+1-N/2} \quad (6.2)$$

with probability $p = \sin^2(\rho/2)$, which can be written, in fact, immediately starting from the integral form (4.10) or using combinatorial arguments to calculate the norm of the particle-number-projected BCS states.

Let us consider now that a number of nucleons, N, are distributed among two single-particle states whose quantum numbers are specified through their angular momenta j_1 and j_2, respectively. The potential entering Eq. (5.1) now has the form

$$\mathcal{V}_{\alpha\beta} = 2G. \quad (6.3)$$

The corresponding energies of the shells are denoted by ϵ_1 and ϵ_2, respectively.

A. Standard BCS

If one neglects the renormalization of the single-particle energies due to the pairing interaction, the energy of the constrained system of N nucleons has the expression

$$E'(N) = \sum_{\alpha} 2(2j_\alpha + 1)(\epsilon_\alpha - \lambda)|V_\alpha|^2 - \frac{|\Delta|^2}{G}, \quad (6.4)$$

with

$$\Delta = \frac{G}{2} \sum_{\alpha} 2(2j_\alpha + 1) U_\alpha V_\alpha, \quad (6.5)$$

$$N = \sum_{\alpha} 2(2j_\alpha + 1)|V_\alpha|^2. \quad (6.6)$$

The condition of minimum energy as a function of the BCS angles can be used to express the BCS angles in terms of the

energy gap Δ and the parameter λ:

$$\begin{pmatrix} |V_\alpha|^2 \\ U_\alpha^2 \end{pmatrix} = \frac{1}{2}\left(1 \mp \frac{\epsilon_\alpha - \lambda}{\sqrt{(\epsilon_\alpha - \lambda)^2 + |\Delta|^2}}\right). \tag{6.7}$$

The energy gap and λ can be found from the self-consistency condition (6.5) and the particle number constraint (6.6):

$$\sum_\alpha \frac{(2j_\alpha + 1)(\epsilon_\alpha - \lambda)}{\sqrt{(\epsilon_\alpha - \lambda)^2 + |\Delta|^2}} = \sum_\alpha (2j_\alpha + 1) - N,$$
$$\frac{G}{2}\sum_\alpha \frac{2j_\alpha + 1}{\sqrt{(\epsilon_\alpha - \lambda)^2 + |\Delta|^2}} = 1. \tag{6.8}$$

The variational problem also constrains the phases. Denoting by φ the phase of the gap parameter

$$\Delta = |\Delta| e^{i\varphi}, \tag{6.9}$$

one successively finds $\arg V_\alpha = \arg \Delta$, or, using the relation (3.7),

$$\psi_\alpha + \frac{\pi}{2} = \varphi. \tag{6.10}$$

The average energy (6.4) is independent of the phase factor of V_α. The absolute scale of the phases, therefore, is not determined.

If the BCS equations admit nontrivial solutions, the system is, by definition, in a superconducting phase, its energy being calculated by Eq. (6.4).

In the case of a single shell, the solution of the above equations has the form

$$\epsilon_1 - \lambda = \tfrac{1}{2}G(2j + 1 - N),$$
$$\Delta^2 = \tfrac{1}{4}G^2 N(4j + 2 - N),$$
$$V_j^2 = \frac{N}{2(2j+1)},$$
$$E'(N) = -\frac{G}{4}N^2.$$

The quasiparticle energy is equal to $\frac{G}{2}(2j + 1)$ while the system energy is obtained by subtracting from $E'(N)$ the contribution of the constraint term:

$$E_{gs}(N) = \epsilon_1 N - \tfrac{1}{4}GN(4j + 2 - N). \tag{6.11}$$

In the BCS theory, therefore, the superconducting state exists for any number of particles. This conclusion, however, is not supported in the particle-number-projected BCS theory. It is not difficult to see that the average energy corresponding to the N-projected BCS state is independent of the BCS angles and phases and equal to

$$E(N) = \epsilon_1 N - \tfrac{1}{4}GN(4j + 4 - N). \tag{6.12}$$

This result can be obtained with the general formulas of the previous sections, where λ is set equal to zero, but also by exploiting the fact that, after projecting the nucleon total number, only the component $\sim(J_+)^{N/2}|0\rangle$ survives in the BCS wave function. The average value of the Hamiltonian $\hat{H}$, corresponding to $\lambda = 0$, for this component provides (6.12). Note that the unprojected BCS state is higher in energy than and the N-projected BCS state.

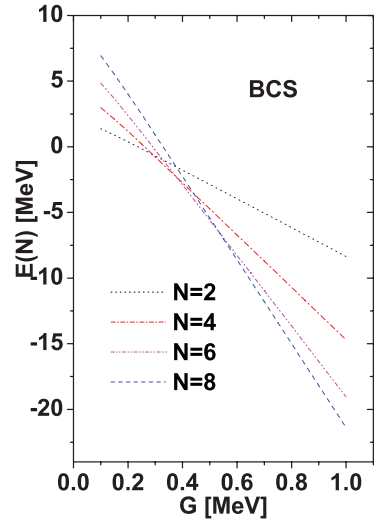

FIG. 1. (Color online) The energy of a system with N nucleons ($N = 2, 4, 6, 8$), obtained within the BCS formalism, plotted as a function of the pairing interaction strength G.

Moreover, the system defined by the Hamiltonian (6.1) restricted to a single shell is exactly solvable, since the components of the Hamiltonian are expressed through the Casimir operator of the quasirotation group, $\hat{J}_\alpha^2$, and the quasispin projection on z axis, $\hat{J}_{\alpha 0}$. In our case, the expression of (6.12) appears to be just the eigenvalue of the pairing Hamiltonian, while the N-projected state is the corresponding eigenfunction.

B. N-projected BCS

Here we consider the case of two-shell calculations.

By using the matrix elements (5.6), (5.13), and (5.14) the system energy calculated as the average value of the pairing Hamiltonian $\hat{H}$ corresponding to the N-projected BCS state is readily obtained.

Making use of the results obtained so far one can calculate the ground-state energies as well as the energy gap. Calculations were successively performed for the standard BCS, the PBCS, and the FBCS formalisms. Also, the exact eigenvalues of $\hat{H}$ have been obtained by diagonalization. The input data in our calculation are

$$j_1 = \tfrac{3}{2}, \quad j_2 = \tfrac{7}{2},$$
$$\epsilon_1 = 1 \text{ MeV}, \quad \epsilon_2 = 1.5 \text{ MeV}. \tag{6.13}$$

For a given N ($= 2, 4, 6, 8$) we solved the BCS equations (6.8) and then calculated the ground-state energy (6.4). Results for energies are plotted, in Fig. 1, as function of the pairing interaction strength. The uncorrelated system has the energy

$$E_{\text{normal}} = N\epsilon_1. \tag{6.14}$$

Alternatively, with the parameters $\rho_1, \rho_2, \psi_1, \psi_2$ determined by the standard BCS approach, the system energy was calculated with the general expression provided by the present formalism with the N-projected state. We conventionally

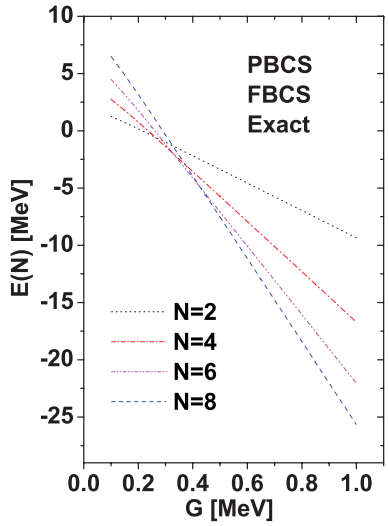

FIG. 2. (Color online) The energy of a system with N nucleons ($N = 2, 4, 6, 8$), obtained within the PBCS formalism, plotted as a function of the pairing interaction strength G. Energies predicted by the PBCS, the FBCS, and diagonalization (Exact) are identical. This is indicated by assigning to the given curves all three labels: PBCS, FBCS, and Exact.

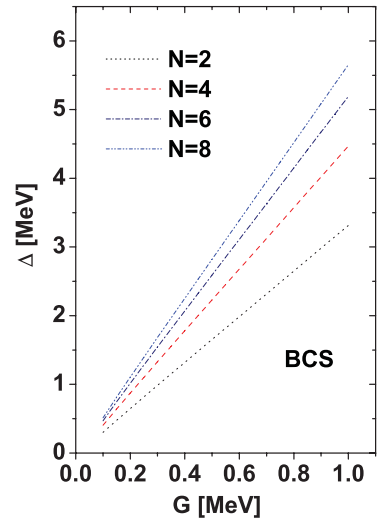

FIG. 3. (Color online) The gap energy for a system with N nucleons ($N = 2, 4, 6, 8$) plotted as a function of the pairing interaction strength G within the standard BCS formalism.

call this approach the projected BCS (PBCS). The resulting energies are represented in Fig. 2 as functions of G.

For each N, further, the energy $E(N)$ given by the N-projection formalism was minimized with respect to the parameters involved in the trial function, i.e., $\rho_1, \rho_2, \psi_1, \psi_2$. It turns out that the ground-state energies provided by PBCS, FBCS, and diagonalization are equal to each other for any G in the range of 0.1–1.0 MeV. The common values were used in Fig. 2, showing the energy dependence on the pairing strength parameter.

The two figures mentioned before exhibit some common features. Energies are decreasing functions of G. They show a linear dependence on G with the slope depending on the total particle number, N. For low values of G, energies are increasing functions of N, while for large pairing strength they are decreasing with N. In the four approaches, the transition from one energy ordering to another is taking place for different values of G. The largest critical G is met for the standard BCS. The superconducting phase is achieved for any $G \geqslant 0.1$. It is remarkable that energies provided by the PBCS and FBCS approaches are the same. For a given set of G and N the ground-state energies obtained in different approaches are ordered as follows:

$$E_{\text{normal}} > E_{BCS} > E_{PBCS} = E_{FBCS}. \tag{6.15}$$

Another observable considered in our study is the energy gap obtained within the standard BCS and the FBCS formalisms, respectively. The results obtained for a fixed N were plotted as a function of G in Figs. 3 and 4, respectively. These figures show a linear dependence of both gaps on G. The split of gaps due to their N dependence is larger for Δ than for $\Delta^{(N)}$. Indeed, according to the numerical results, $\Delta(N = 8) - \Delta(N = 2)$ is equal to 0.212 and 2.338 MeV for G equal to 0.1 and 1.0 MeV, respectively, while $\Delta^{(8)} - \Delta^{(2)}$ for $G = 0.1$ and 1.0 MeV amounts to 0.146 and 1.633 MeV, respectively. Note that for a given set of N and G we have $\Delta > \Delta^{(N)}$. Since the energy gap might be looked at as a measure of superconductivity one may expect that the superconductivity effects are more pronounced in the PBCS and FBCS than in the BCS.

The Hamiltonian $\hat{H}$ can be diagonalized in a basis of definite number of particles, N:

$$|N_1, N_2\rangle = C_{N_1 N_2}(c_1^\dagger d_{\tilde{1}}^\dagger)^{N_1/2}(c_2^\dagger d_{\tilde{2}}^\dagger)^{N_2/2}|0\rangle, \quad N_1 + N_2 = N, \tag{6.16}$$

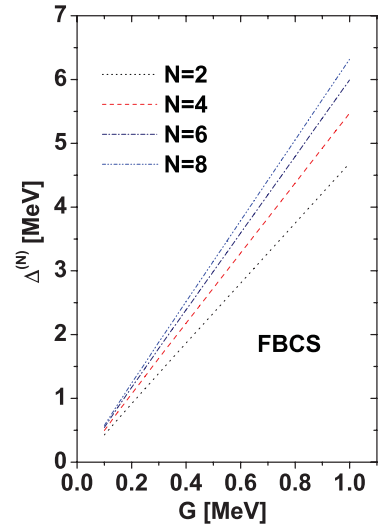

FIG. 4. (Color online) The gap energy for a system with N nucleons ($N = 2, 4, 6, 8$) plotted as a function of the pairing interaction strength G within the standard FBCS formalism. The gap function is defined by Eq. (5.11).

with $C_{N_1N_2}$ standing for the normalization constant. The matrix elements of H in this basis have simple expressions:

$$\begin{aligned}
&\langle N_1, N_2|H|N_1, N_2\rangle \\
&\quad = \epsilon_1 N_1 + \epsilon_2 N_2 - \frac{G}{4}[N_1(4j_1 + 4 - N_1) \\
&\qquad + N_2(4j_2 + 4 - N_2)], \\
&\langle N_1 + 2, N_2 - 2|H|N_1, N_2\rangle \\
&\quad = -\frac{G}{4}[(N_1 + 2)N_2(4j_1 + 2 - N_1)(4j_2 + 4 - N_2)]^{1/2}, \\
&\langle N_1 - 2, N_2 + 2|H|N_1, N_2\rangle \\
&\quad = -\frac{G}{4}[N_1(N_2 + 2)(4j_1 + 4 - N_1)(4j_2 + 2 - N_2)]^{1/2}.
\end{aligned} \tag{6.17}$$

For each N and a fixed G, we diagonalized the above matrix and depicted the lowest eigenvalues. Further, these were compared with the energies provided by the FBCS and the PBCS formalisms. In this way we found out that the three sets of energies are identical. This is a nice example of when the solution of two variational principle equations reproduce the exact ground-state energy. However, in a realistic single-particle space and, moreover, when an isospin-invariant Hamiltonian is instead considered, this feature does not necessarily show up.

Let us now say a few words about the relationship of the present formalism and that from Ref. [38]. Therein the variational state is obtained by applying a particular rotation in the isospin space to the BCS state associated with a system with $N = Z$. The basic state [Eq. (2.3) from the quoted reference] is however different from the one used in the present work (3.2), although the corresponding BV transformation differs only by a phase factor "i" in the coefficient V. The expression e^{-iF} chosen in the present work has the advantage of being a rotation and, moreover, many of the matrix elements have a clear interpretation. The additional rotation appearing in the expression of the generalized BCS state is necessary for a realistic treatment of the Hamiltonian used in the mentioned work, which has a complex structure and therefore is different from the one used here. There, the matrix elements are obtained by brute-force calculation by expanding the exponentials and then performing the tedious commutators involving monomials and binomials of creation and annihilation single-fermion operators, whereas here the particle number projection is achieved by using the Cauchy theorem for integrating over the gauge angle. Moreover, in order to do that, the operators whose matrix elements are to be evaluated are exponentiated, which results in simplifying significantly the manipulation efforts. Only in this way can the matrix elements be expressed in terms of the norms of the projected states. In turn, these satisfy a recursive formula which, as a matter of fact, generalizes the one of Ref. [6], obtained for like-nucleon pairing. It is remarkable that despite its generalizing feature our recursion expression is simpler than the one of Ref. [6]. We stress again that this is actually the main objective of the present paper. We just mention that, by contrast, even for the single j case considered in Ref. [38] the expressions are quite complicated. Extension of the present formalism to isoscalar Hamiltonians requires of course a variational state of a more complex structure. Then combining the results of Ref. [38] and those from here we hope to obtain the eigenvalues of the chosen Hamiltonian in the space of states with restored gauge and isospin symmetries for a large single-particle space. We hope we shall be able to report on this project in the near future.

VII. CONCLUSIONS

Many interesting properties of pn pairing have been derived using for the BCS function of the form (3.1). After making use of the factorization described in Sec. I, one finds that the function (3.1) for a fixed α represents the coherent state of the SU(2) group generated by $J_{\alpha\mu}$. Our attention was focused on the nucleon-number-projected BCS. Since any matrix element can be expressed in terms of the norms of the involved states, we started with the norm calculation. One of the main results of the present paper is the recursive formula for these norms. By using this equation the norm of a projected state with N particles is related to the norms of the N'-projected states with $N' < N$. For pairing interaction of like nucleons, a similar recursion formula was obtained in Ref. [6]. The difference between the two recursion formulas is that there the recursion is operating in two dimensions and two indices are iterated, while here only one index is involved in the recursion.

To prove the usefulness of the obtained recursion formula several matrix elements have been evaluated. The one for the proton-neutron pairing operator of a given shell is interpreted as a spectroscopic factor for a deuteron transfer reaction. Being guided by the analogy with like-nucleon pairing we defined a quantity which might be a measure for the energy gap in the particle-number-projected picture. Also, we calculated the occupation probability for a given state with a proton-neutron pair. In the Appendix the matrix element involved in the width of an α-decay process is analytically expressed. Also, the matrix element for the two-body proton-neutron interaction in the particle-particle channel between the states associated with the mother and daughter nuclei involved in a double-β Fermi decay are obtained in a compact form.

Using a Hamiltonian including a mean-field term and a proton-neutron pairing interaction we calculated the system energy as a function of the particle number N and the parameters ρ_α, ψ_α defining the unprojected BCS wave function. Since many features of the paired system can be found also in a restricted single-particle space we discussed the simple cases of one and two single-particle states. Since the energy associated with a single j and the N-projected picture is constant with respect to the BCS parameters we concluded that for this case a superconducting phase cannot be reached. However, the case of two j is suitable for studying the pairing properties in both the standard BCS and projected BCS formalisms. In the later situation we considered both cases when the variation is performed before and after projection. In the two-level situation we have proved that the ground-state energy provided by the PBCS and the FBCS are the same and moreover equal to the exact ground-state energy obtained by diagonalization. It is an open question whether this feature

is caused by the restricted single-particle space or by the particular choice of the model many-body Hamiltonian.

One of the evident limitations of our formalism consists in the fact that the trial BCS unprojected function allows us to describe only nuclei with $N = Z$. This feature can, however, be improved by adding two factors accounting for the proton-proton and neutron-neutron pairing, respectively, to (3.1).

As an imminent project for the near future we also mention the extension of our formalism to isospin-preserving Hamiltonians. In the second step of the formalism development we shall attempt to include in our study proton-neutron $T = 0$ pairing as well as isospin projection. This plan is, in fact, a reflection of our belief that a new and powerful technical result might be decisive in unveiling new properties of the paired proton-neutron system.

ACKNOWLEDGMENTS

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APPENDIX: MATRIX ELEMENTS OF DIFFERENT FINAL AND INITIAL PARTICLE-NUMBER-PROJECTED BCS STATES

In various applications matrix elements of operators between two different BCS states are frequently encountered. In the case of projected BCS, such matrix elements are calculated in the manner described in Sec. V. Here we derive formulas for $\langle BCS_f, N_f|O|BCS_i, N_i\rangle$ for $O = 1$, $J_{\pm\alpha}$, $J_{\pm\alpha}J_{\pm\beta}$, and $J_{\mp\alpha}J_{\pm\beta}$ with different BCS angles of the final and initial states.

We start from the diagonal in particle number overlap,

$$\begin{aligned}\langle BCS_f, N|BCS_i, N\rangle &= Q_f^{-1/2}(N)\langle BCS_f|BCS_i, N\rangle \\ &= Q_f^{-1/2}(N)Q_i^{-1/2}(N)Q_{fi}(N),\end{aligned}$$

where $Q_f(N)$ and $Q_i(N)$ are the diagonal Q functions defined for the final- and initial-state BCS angles $(\rho'_\alpha, \psi'_\alpha)$ and $(\rho_\alpha, \psi_\alpha)$, respectively. Calculations similar to those carried out in Sec. V give the off-diagonal Q function

$$\begin{aligned}Q_{\rm fi}(N) = \int_C \frac{d\zeta}{2\pi i}\frac{1}{\zeta^{N+1}}\prod_\alpha[&\cos(\rho'_\alpha/2)\cos(\rho_\alpha/2) \\ &+ \zeta^2\exp(i\psi'_\alpha - i\psi_\alpha)\sin(\rho'_\alpha/2)\sin(\rho_\alpha/2)]^{2j_\alpha+1}.\end{aligned} \tag{A1}$$

Integrating by parts and expanding into a series in ζ or $1/\zeta$, we obtain the recursion for the calculation of this function:

$$\begin{aligned}Q_{\rm fi}(N) &= \sum_\alpha Q^\alpha_{\rm fi}(N), \\ Q^\alpha_{\rm fi}(N) &= \frac{\Omega_\alpha}{N}\sum_{n=1}^{N/2}(-)^{n+1}[\exp(i\psi'_\alpha - i\psi_\alpha)\tan(\rho'_\alpha/2) \\ &\quad\times\tan(\rho_\alpha/2)]^n Q_{\rm fi}(N-2n)\end{aligned} \tag{A2}$$

$$\begin{aligned}&= \frac{\Omega_\alpha}{\Omega - N}\sum_{n=1}^{(\Omega-N)/2}(-)^{n+1}[\exp(-i\psi'_\alpha + i\psi_\alpha)\cot(\rho'_\alpha/2) \\ &\quad\times\cot(\rho_\alpha/2)]^n Q_{\rm fi}(N+2n).\end{aligned} \tag{A3}$$

The boundary conditions follow from (A1):

$$\begin{aligned}Q_{\rm fi}(0) &= \prod_\alpha[\cos(\rho'_\alpha/2)\cos(\rho_\alpha/2)]^{2j_\alpha+1}, \\ Q_{\rm fi}(\Omega) &= \prod_\alpha[\exp(i\psi'_\alpha - i\psi_\alpha)\sin(\rho'_\alpha/2)\sin(\rho_\alpha/2)]^{2j_\alpha+1}.\end{aligned}$$

As in the case of the function $Q(N)$, $Q_{\rm fi}(N)$ vanishes outside the interval $(0, \Omega)$ and for odd N. In the limit where the angles in the initial and final BCS states coincide, we recover the result for $Q(N)$. In particular, $Q_{ff}(N) = Q_f(N)$ and $Q_{ii}(N) = Q_i(N)$. $Q^\alpha_{\rm fi}(N)$ vanishes outside the interval $(2, \Omega - 2)$.

Now, consider the two-fermion gap function

$$\begin{aligned}\langle J_{\alpha+}\rangle_{\rm fi} &= \langle BCS_f, N+2|J_{\alpha+}|BCS_i, N\rangle \\ &= Q_f^{-1/2}(N+2)\langle BCS_f|J_{\alpha+}|BCS_i, N\rangle.\end{aligned}$$

The calculation is performed using the representation of $J_{\alpha+}$ in the exponential form

$$J_{\alpha+} = -i\frac{d}{dx}\exp(iJ_{\alpha+}x)|_{x=0}$$

and Eq. (3.15). A similar representation is used for the other quasispin components. After some algebraic manipulations, we obtain

$$\begin{aligned}\langle J_{\alpha+}\rangle_{\rm fi} &= -iQ_f^{-1/2}(N+2)Q_i^{-1/2}(N)\frac{1}{2\sqrt{2}}(N+2)\exp(i\psi_\alpha) \\ &\quad\times\cot(\rho_\alpha/2)Q^\alpha_{\rm fi}(N+2),\end{aligned} \tag{A4}$$

$$\begin{aligned}\langle J_{\alpha 0}\rangle_{\rm fi} &= Q_f^{-1/2}(N)Q_i^{-1/2}(N) \\ &\quad\times\left[\frac{N}{2}Q^\alpha_{\rm fi}(N) - (j_\alpha + 1/2)Q_{\rm fi}(N)\right].\end{aligned} \tag{A5}$$

Summing the last equation over α one arrives at

$$2\sum_\alpha\langle J_{0\alpha}\rangle_{\rm fi} = Q_f^{-1/2}(N)Q_i^{-1/2}(N)Q_{\rm fi}(N)\left(N - \frac{1}{2}\Omega\right),$$

which is consistent with the definition for particle number operator, Eq. (4.3). The expression for $\langle J_{\alpha-}\rangle_{\rm fi}$ is obtained by complex conjugation (A4).

Consider now the four-fermion gap function

$$\langle J_{\alpha+}J_{\beta+}\rangle_{\rm fi} = \langle BCS_f, N+4|J_{\alpha+}J_{\beta+}|BCS_i, N\rangle.$$

This matrix element represents the width of the α decay of the mother nucleus in the state $|BCS_f, N+1\rangle$ to the daughter nucleus in the state $|BCS_i, N_f\rangle$. Also, based on this matrix element one may define the spectroscopic factor of a reaction which removes an α particle from the states α and β. In other words, squaring this matrix element one obtains the occupation probabilities of the states α and β with proton-neutron pairs. The calculation uses the representation

$$J_{\alpha+}J_{\beta+} = -\frac{d}{dx}\frac{d}{dy}\exp(iJ_{\alpha+}x + iJ_{\beta+}y)|_{x=y=0}$$

and the method of Sec. II. For $\alpha \neq \beta$, we obtain

$$\langle J_{\alpha+}J_{\beta+}\rangle_{\rm fi} = -Q_f^{-1/2}(N+4)Q_i^{-1/2}(N)\frac{1}{4}(N+2)[(2j_\beta+1)Q^\alpha_{\rm fi}(N+2)-(2j_\alpha+1)Q^\beta_{\rm fi}(N+2)] \times \frac{\exp(i\psi'_\beta+i\psi'_\alpha)\tan(\rho'_\alpha/2)\tan(\rho'_\beta/2)}{\exp(i\psi'_\alpha-i\psi_\alpha)\tan(\rho'_\alpha/2)\tan(\rho_\alpha/2)-\exp(i\psi'_\beta-i\psi_\beta)\tan(\rho'_\beta/2)\tan(\rho_\beta/2)}. \quad (A6)$$

A similar expression is obtained for the matrix element

$$\begin{aligned}\langle J_{\alpha+}J_{\beta-}\rangle_{\rm fi} &= \langle BCS_f, N|J_{\alpha+}J_{\beta-}|BCS_i, N\rangle \\ &= -Q_f^{-1/2}(N)Q_i^{-1/2}(N)\frac{1}{4}N[(2j_\beta+1)Q^\alpha_{\rm fi}(N)-(2j_\alpha+1)Q^\beta_{\rm fi}(N)] \\ &\quad\times\frac{\exp(i\psi'_\beta-i\psi_\alpha)\tan(\rho'_\beta/2)\tan(\rho_\alpha/2)}{\exp(i\psi'_\alpha-i\psi_\alpha)\tan(\rho'_\alpha/2)\tan(\rho_\alpha/2)-\exp(i\psi'_\beta-i\psi_\beta)\tan(\rho'_\beta/2)\tan(\rho_\beta/2)}. \quad (A7)\end{aligned}$$

We may ask ourselves how that situation may appear. The answer is offered by the double-β decay with and without neutrinos in the final state. Indeed, in such a process the nucleus $|\mathcal{N}, Z\rangle$ goes to the nucleus $|\mathcal{N}-2, Z+2\rangle$, two electrons and either two or zero antineutrinos respectively, where $\mathcal{N}$ and Z denote the neutron and the proton number of the initial system. The mentioned states are described by different sets of BCS angles and phases but have equal number of nucleons. As a matter of fact the two-body interaction whose matrix element is calculated is nothing else but the particle-particle interaction of the Fermi type. These comments prove that to calculate such a matrix element is an important step in describing some important physical processes.

The average (A6) is symmetric under interchange of the indices and $\langle J_{\alpha+}J_{\beta-}\rangle_{\rm fi} = \langle J_{\beta-}J_{\alpha+}\rangle_{\rm fi}$. Complex conjugation of (A6) allows us to find $\langle J_{\alpha-}J_{\beta-}\rangle_{\rm fi}$.

When shells are the same, the result is as follows:

$$\begin{aligned}\langle J_{\alpha+}J_{\alpha+}\rangle_{\rm fi} &= -Q_f^{-1/2}(N+4)Q_f^{-1/2}(N)\frac{j_\alpha}{2}\exp(i\psi_\alpha+i\psi'_\alpha)\tan(\rho'_\alpha/2)\cot(\rho_\alpha/2) \\ &\quad\times\sum_{n=0}^{N/2}(-)^n[\exp(i\psi'_\alpha-i\psi_\alpha)\tan(\rho'_\alpha/2)\tan(\rho_\alpha/2)]^n(N+2-2n)Q^\alpha_{\rm fi}(N+2-2n) \quad (A8) \\ &= -Q_f^{-1/2}(N+4)Q_i^{-1/2}(N)j_\alpha(2j_\alpha+1)\exp(2i\psi'_\alpha)\tan^2(\rho'_\alpha/2) \\ &\quad\times\sum_{n=0}^{N/2}(-)^n[\exp(i\psi'_\alpha-i\psi_\alpha)\tan(\rho'_\alpha/2)\tan(\rho_\alpha/2)]^n(n+1)Q_{\rm fi}(N-2n), \quad (A9)\end{aligned}$$

$$\langle J_{\alpha+}J_{\alpha-}\rangle_{\rm fi} = -Q_f^{-1/2}(N)Q_i^{-1/2}(N)\left\{\frac{N}{2}Q^\alpha_{\rm fi}(N)+(j_\alpha+1/2)\sum_{n=1}^{N/2}(-)^{n+1}[\exp(i\psi'_\alpha-i\psi_\alpha)\tan(\rho'_\alpha/2)\tan(\rho_\alpha/2)]^n \times(2nj_\alpha-1)Q_{\rm fi}(N-2n)\right\}. \quad (A10)$$

The representations (A8) and (A9) are equivalent.

The formalism also provides an expression for the average as a sum over the quantum numbers α for a fixed number of particles as well. However, the number of shells is usually much larger than N, and the ratio between Ω and N indicates the accuracy of the solution of the variational problem. The higher the ratio, the higher the accuracy. For this reason, the summation over the number of particles is easier from the computational point of view, and it is therefore preferable. Also, the recursive computation of the function $Q_{\rm fi}(N)$ starting from small numbers of particles is simpler.

The function $Q_{\rm fi}(N)$ can be written in the form [38]

$$Q_{\rm fi}(N) = \sum_{N_1+N_2+\ldots=N}\prod_\alpha\frac{(\Omega_\alpha/2)!}{(\Omega_\alpha/2-N_\alpha/2)!(N_\alpha/2)!}[\exp(-i\psi'_\alpha+i\psi_\alpha)\sin(\rho'_\alpha/2)\sin(\rho_\alpha/2)]^{N_\alpha/2}[\cos(\rho'_\alpha/2)\cos(\rho_\alpha/2)]^{\Omega_\alpha/2-N_\alpha/2}. \quad (A11)$$

Here the summation is over all sets of even occupation numbers N_α, whose sum is the total number of particles. In the special case of a single shell, we reproduce Eq. (6.2).

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