Some exact results for the particle number projected BCS approach of the isovector proton-neutron pairing

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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 step of iteration. An illustrative example is numerically considered in a restricted single particle space. Some specific features for the standard BCS, the projection after variation approach as well as for the variation after projection formalism, are pointed out.

I. INTRODUCTION

Short after the theory of superconductivity \cite{1, 2} showed up it has been realized \cite{2} that such a formalism might work also for nuclear systems although the constituents number 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 in the average. Amazingly the pairing force and the emerging seniority scheme has been introduced much earlier, by Racah \cite{1}. A serious question arose, namely to what extent the 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 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. The particle number projection has been first considered by Bayman in Ref. \cite{5}. There the averages of the Hamiltonian, including the mean field and pairing terms, and of particle number operator are expressed as functions of some residuum integrals which where 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. \cite{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 levels pairing model \cite{7}.

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

Although not as extensively, the Cooper pairs of one proton and one neutron have also been investigated \cite{12, 13}. The results reported there demonstrate that the generalized Bogoliubov-Valatin (BV) transformation including \textit{pp}, \textit{nn} and \textit{pn} pairing is appropriate for treating

*https://sites.google.com/site/saveitep/*
the pairing correlations in a self-consistent way, in spite of some earlier pessimistic views on this issue \cite{19,20}. Note that in a generalized (BV) formalism both the total number of nucleons, the isospin third component (T3) and isospin (T) are not conserved. Therefore a simultaneous projection for all the three quantum numbers is necessary. This type of projection has been considered by several authors both numerically and analytically \cite{21,22}. The integrability of a \pm pairing model was treated in Refs. \cite{23,24} by different methods. Thus the pairing Hamiltonian introduced by Richardson in Ref. \cite{25} 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 \cite{26}. A different method is applied, in Ref. \cite{24}, to the same Richardson model which includes isospin-symmetry breaking terms.

It seems that the common mathematical content with the above pairing correlated system is a serious ground for considering the pairing effect for other systems. Pairing forces acting among the quarks in two-color QCD matter lead to the color superconductivity \cite{26,27}, as also confirmed by simulations in lattice gauge theories \cite{28}. Superconductivity of metallic nanoparticles is discussed in Refs. \cite{29,30,31}. Due to its paramount importance it is worth simplifying the formalism applied to other degrees of freedom following the successful path used for pairing of alike nucleons.

In this context the present paper considers the isovector \pm 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 Section 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 operator. This is shown in Section III. The particle number projected function is described in Section IV. Analytical results of the average values of various interaction terms are given in Section V. Numerical results for a pairing Hamiltonian considered in a restricted single particle space are given in Section VI. The final conclusions are collected in Section VII.

II. FACTORIZATION OF THE ROTATION OPERATOR

In the theory of superconductivity bi-linear 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 wave function is given by real angle \( \theta \) and the real unit vector \( \mathbf{n} \)

\[
\Psi \to \Psi' = \exp(-i\theta \mathbf{n}\mathbf{J})\Psi,
\]

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 \( \theta, \mathbf{n} \) from Eq. \( \eqref{2.1} \) and those denoted by \( \alpha_\mu \) and \( \beta_\mu (\mu = \pm, 0) \) which define two independent factorized forms for the same rotation operator

\[
\exp(-i\theta \mathbf{n}\mathbf{J}) \equiv U = \exp(i\theta n_- J_+ - i\theta n_0 J_0 + i\theta n_+ J_-)
= \exp(i\alpha_- J_+) \exp(-i\alpha_0 J_0) \exp(i\alpha_+ J_-)
= \exp(i\beta_+ J_-) \exp(-i\beta_0 J_0) \exp(i\beta_- J_+).
\]

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

\[
\mathbf{n}\mathbf{J} = -n_- J_+ + n_0 J_0 - n_+ J_-,
\]

where

\[
J_+ = \frac{1}{\sqrt{2}}(J_1 + iJ_2),
J_- = \frac{1}{\sqrt{2}}(J_1 - iJ_2),
J_0 = J_3.
\]

Throughout the present paper the used notations are consistent with those of Ref. \cite{32}. The spherical components of the unit vector are:

\[
n_\pm = \pm \frac{1}{\sqrt{2}} \sin(\Theta) \exp(\pm i\Phi),
n_0 = \cos(\Theta),
\]

where \( \Theta \) and \( \Phi \) are the polar and azimuthal angles. The unit length of the vector \( \mathbf{n} \) implies, in the cyclic basis,

\[
-2n_- n_+ + n_0^2 = 1.
\]

The decomposition \( \eqref{2.2} \) 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 between the parameters \( \theta, \mathbf{n} \) and \( \alpha_\mu \) can be found by taking the derivative over the \( \theta \) of the left and right sides in Eq. \( \eqref{2.2} \) and using the commutation relations for the rotation generators. The derivative over \( \theta \) gives

\[
(i n_- J_+ - i n_0 J_0 + i n_+ J_-) \exp(-i\theta \mathbf{n}\mathbf{J}) =
\]

\[
\alpha_- J_+ \exp(i\alpha_0 J_0) \exp(-i\alpha_0 J_0) \exp(i\alpha_+ J_-)
\]

\[
-\alpha_0 \exp(i\alpha_0 J_0) J_0 \exp(-i\alpha_0 J_0) \exp(i\alpha_+ J_-)
\]

\[
+\alpha_+ J_- \exp(i\alpha_0 J_0) \exp(-i\alpha_0 J_0) \exp(i\alpha_+ J_-).
\]
Here the symbol \("n"\) stands for the derivative with respect to the variable \(\theta\). Using the commutation relations satisfied by the angular momentum components \(\alpha\)

\[
\begin{align*}
[J_+, J_-] &= -J_0, \\
[J_\pm, J_0] &= \mp J_\pm.
\end{align*}
\]

one finds

\[
\begin{align*}
\exp(i\alpha_- J_0)\exp(-i\alpha_+ J_0) &= J_0 - i\alpha_- J_+, \\
\exp(-i\alpha_0 J_0)\exp(i\alpha_0 J_0) &= J_\pm \exp(i\alpha_0), \\
\exp(i\alpha_- J_0)\exp(-i\alpha_+ J_0) &= J_- - i\alpha_- J_0 - \frac{\alpha^2}{2} J_+.
\end{align*}
\]

In deriving the above relations we made use of the following equation:

\[
e^A B e^{-A} = \sum_{k=0}^{\infty} \frac{1}{k!} [A_1, [A_2, [\ldots [A_k B] \ldots]]].
\]

which holds for any operators \(A\) and \(B\). One thus arrives at the equation

\[
in_- J_+ - in_0 J_0 + in_+ J_- = i\alpha'_- J_+ - i\alpha'_0 (J_0 - i\alpha_- J_+) + i\alpha'_+ \exp(i\alpha_0) (J_- - i\alpha_- J_0 - \frac{\alpha^2}{2} J_+), \quad (2.9)
\]

that can be split into three equations

\[
\begin{align*}
n_- &= \alpha'_- + i\alpha'_0 \alpha_- - \alpha'_+ \exp(i\alpha_0) \frac{\alpha^2}{2}, \\
n_0 &= \alpha'_0 + i\alpha'_+ \exp(i\alpha_0) \alpha_-, \\
n_+ &= \alpha'_+ \exp(i\alpha_0),
\end{align*}
\]

which can further be brought to the equivalent form

\[
\begin{align*}
n_- &= \alpha'_- + in_0 \alpha_- + \frac{n\alpha^2}{2}, \\
n_0 &= \alpha'_0 + in_+ \alpha_- = \alpha'_-, \\
n_+ &= \alpha'_+ \exp(i\alpha_0).
\end{align*}
\]

Using the boundary conditions

\[
\alpha_-(0) = \alpha_0(0) = \alpha_+(0) = 0,
\]

we obtain

\[
\begin{align*}
\alpha_\pm(\theta) &= \frac{n\pm 2 \tan(\theta/2)}{1 + i n_0 \tan(\theta/2)}, \quad (2.12) \\
\alpha_0(\theta) &= -2i \ln(\cos(\theta/2) + in_0 \sin(\theta/2)). \quad (2.13)
\end{align*}
\]

The result for the functions \(\alpha_\mu(\theta)\), depends only on the commutation relations of \(J_\mu\) 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 \(J_\mu\) by the Pauli matrices divided by 2. Next, we expand the left and right sides of the expression \((2.2)\) in the parameters \(\theta\) and \(\alpha_\mu\). The decomposition over \(\alpha_\pm\) is necessarily truncated at the terms linear in \(\alpha_\pm\) due to the equation \(J_0^2 = 0\) 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 equations \((2.12)\) and \((2.13)\).
operators $J_\mu$. These relations are, however, simple:

$$\beta_\pm = -\alpha_\pm^*,$$  \hspace{1cm} (2.16)

$$\beta_0 = \alpha_0^*.$$  \hspace{1cm} (2.17)

Equations (2.16) and (2.17) are the necessary and sufficient in order that the operator $U$ is unitary. They are therefore valid for real $\theta$ and for real unit vectors $n$, that is for pure rotation. These equations cannot be continued analytically to the complex values of $\theta$ and $n$, because they involve the operation of complex conjugation. In the case of complex rotations, one should return to equations (2.13) and (2.14). We express the complex parameters $\theta$ and $n$ through $\alpha_\mu$, and substitute these expressions in formulas (2.13) and (2.15). Simple calculations give

$$\beta_\pm = \frac{\alpha_\pm \exp(i\alpha_0)}{1 + \frac{1}{2} \alpha_+ \alpha_- \exp(i\alpha_0)},$$  \hspace{1cm} (2.18)

$$\beta_0 = \alpha_0 + 2i \ln\left(1 + \frac{1}{2} \alpha_+ \alpha_- \exp(i\alpha_0)\right).$$  \hspace{1cm} (2.19)

These formulas establish the connection between arbitrary complex parameters $\alpha_\mu$ and $\beta_\mu$. The inverse relations have the form

$$\alpha_\pm = \frac{\beta_\pm \exp(-i\beta_0)}{1 + \frac{1}{2} \beta_+ \beta_- \exp(-i\beta_0)},$$  \hspace{1cm} (2.20)

$$\alpha_0 = \beta_0 - 2i \left(1 + \frac{1}{2} \beta_+ \beta_- \exp(-i\beta_0)\right).$$  \hspace{1cm} (2.21)

The factorized expression of any rotation like operator is known in the literature as the Baker-Cambell-Haussdorf formula. The general necessary conditions which make this factorization possible are discussed in Ref. [33].

Inverse relations allowing de-factorization of the rotation look as follows:

$$\cos(\theta/2) = \cos(\alpha_0/2) + \frac{1}{4} \alpha_+ \alpha_- \exp(i\alpha_0/2)$$

$$= \cos(\beta_0/2) + \frac{1}{4} \beta_+ \beta_- \exp(-i\beta_0/2),$$

$$n_\pm \sin(\theta/2) = \frac{1}{2} \alpha_\pm \exp(i\alpha_0/2)$$

$$= \frac{1}{2} \beta_\pm \exp(-i\beta_0/2),$$  \hspace{1cm} (2.22)

$$n_0 \sin(\theta/2) = \sin(\alpha_0/2) + \frac{i}{4} \alpha_+ \alpha_- \exp(i\alpha_0/2)$$

$$= \sin(\beta_0/2) + \frac{i}{4} \beta_+ \beta_- \exp(-i\beta_0/2).$$

**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

$$|BCS\rangle = e^{-iF}|0\rangle,$$  \hspace{1cm} (3.1)

where

$$F = \frac{1}{\sqrt{2}} \sum_\alpha \left( z_\alpha e^{i\alpha_m} d^\dagger_\alpha \bar{d}_{\alpha,m} + z_\alpha^* d_\alpha c_{\alpha,m} \right)$$  \hspace{1cm} (3.2)

is a Hermitian operator while $|0\rangle$ denotes the bare vacuum state. Here, $c^\dagger_\alpha$ and $d^\dagger_\alpha$ are particle creation operators for protons and neutrons respectively, $\alpha$ is the index numbering shells. For example, in a spherical shell model $\alpha$ 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. $\bar{d}_{\alpha,m}$ denotes the time reversal sub-state: $d^\dagger_\alpha \bar{d}_{\alpha,m} = (-)^{l-m} d^\dagger_\alpha \bar{d}_{\alpha,-m}$. For alike nucleons in Ref. [34] and for a generalized $pn$ pairing interaction in Ref. [22] analogous, otherwise different, unitary transformations have been used.

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

$$e^{-iF} c^\dagger_\alpha e^{iF} = c^\dagger_\alpha e^{-iF} d^\dagger_\alpha c_{\alpha,m} e^{iF} = \bar{d}_{\alpha,m}.$$  \hspace{1cm} (3.3)

with:

$$c^\dagger_\alpha = \cos\left(\frac{|z_\alpha|}{\sqrt{2}}\right) c^\dagger_\alpha - i \frac{|z_\alpha^*|}{|z_\alpha|} \sin\left(\frac{|z_\alpha|}{\sqrt{2}}\right) d^\dagger_\alpha,$$

$$d^\dagger_\alpha = \cos\left(\frac{|z_\alpha|}{\sqrt{2}}\right) d^\dagger_\alpha - i \frac{|z_\alpha^*|}{|z_\alpha|} \sin\left(\frac{|z_\alpha|}{\sqrt{2}}\right) e^{i\alpha_m} c_{\alpha,m}.$$  \hspace{1cm} (3.4)

We recognize here the Bogoliubov-Valatin (BV) transformation:

$$c^\dagger_\alpha = U^\dagger_\alpha c^\dagger_\alpha - V^\dagger_\alpha d^\dagger_\alpha,$$

$$d^\dagger_\alpha = U^\dagger_\alpha d^\dagger_\alpha - V^\dagger_\alpha c_{\alpha,m}.$$  \hspace{1cm} (3.5)

Using the polar representation of the complex variable $z$,

$$z_\alpha = \frac{1}{\sqrt{2}} \rho_\alpha e^{i\psi_\alpha},$$  \hspace{1cm} (3.6)

the occupation and non-occupation probability coefficients, $V$ and $U$ respectively, are expressed as follows:

$$U_\alpha^\tau = \cos\left(\frac{|\rho_\alpha|}{2}\right),$$

$$V_\alpha^\tau = e^{i(\psi_\alpha + \frac{\pi}{2})} \sin\left(\frac{|\rho_\alpha|}{2}\right), \tau = p, n,$$  \hspace{1cm} (3.7)

The complex variable $z_\alpha$ can be interpreted as the $\mu = -1$ component of a representative vector from the associated classical phase space. From Eq. (3.5) it comes out that the BV transformation coefficients satisfy the normalization conditions:

$$U_\alpha^2 + |V_\alpha|^2 = 1,$$  \hspace{1cm} (3.8)
which assure that the quasiparticle operators obey anti-
commutation relations specific to fermions. Since $U_n^p = U_n^p$ and $V_n^p = V_n^n$, in what follows we shall omit the
isospin index for the BV transformation coefficients.
Applying the operator $\exp(-iF)$ on the obvious equations $c_{am}|0\rangle = d_{am}|0\rangle = 0$ one obtains $c_{am}|\text{BCS}\rangle = d_{am}|\text{BCS}\rangle = 0$, 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 bi-linear operators

\[
J_{\alpha+} = -\frac{1}{\sqrt{2}} \sum_m c_{am}^\dagger d_{am}, \\
J_{\alpha-} = -\frac{1}{\sqrt{2}} \sum_m c_{am} d_{am}, \\
J_{\alpha0} = \frac{1}{2} \sum_m (c_{am}^\dagger c_{am} - d_{am}^\dagger d_{am}),
\]

which satisfy the $SU(2)$ algebra commutation relations (cf. Eqs. (2.7)):

\[
[J_{\alpha+}, J_{\beta-}] = -\delta_{\alpha\beta} J_{\alpha0}, \\
[J_{\alpha-}, J_{\beta0}] = \mp\delta_{\alpha\beta} J_{\alpha\pm}.
\]  
(3.12)

We conventionally call these operators as quasispin oper-
ators. Indeed if we replace the $d$ operators by $c$ the re-
sulting algebra defines the proton seniority states. More-
over replacing the $c$ operators by $d$ one obtains the neu-
tron quasipin algebra which defines the neutron seniority scheme. Although there is a danger of mixing them up with angular momentum operator we use the nota-
tion $J$ for the quasipin algebra operators. Actually the $pn$
pairing operators and the total number of nucleons form a representation of the $SU(2)$ algebra which is differ-
ent from that generated by angular momentum com-
ponents. Due to Eq. (3.12), the transformation $\exp(-iF)$ ac-
tquires the significance of a quasirotation. Within this con-
text the quasiparticle operators appear to be the re-

sult of a quasifraction applied to the creation and anni-
hilation particle operators.

It is worth mentioning some useful properties: $J_{\alpha\pm} = \pm J_{\alpha\mp}$, $J_{\alpha0}$ 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

\[
J_{\alpha-}|0\rangle = 0, \\
J_{\alpha0}|0\rangle = -(j_\alpha + \frac{1}{2})|0\rangle.
\]

For a given $\alpha$ the eigenstates of the proton-neutron pair-
ing Hamiltonian in the restricted single particle space
can be expressed in terms of the irreducible representa-
tions of the $SU(2)$ group. These are the states $|J_\alpha, J_{\alpha0}\rangle$
which are simultaneous eigenstates for the operators $J_\alpha^2$ and $J_{\alpha0}$. The interpretation of the quasispin comes out from the following obvious equations:

\[
\begin{align*}
J_{\alpha-}|J_\alpha, -J_{\alpha0}\rangle &= 0, \\
J_{\alpha0}|J_\alpha, J_{\alpha0}\rangle &= J_{\alpha0}|J_\alpha, J_{\alpha0}\rangle \\
&= \left(\frac{N}{2} - \frac{1}{2}(2j_\alpha + 1)\right)|J_\alpha, J_{\alpha0}\rangle, \\
J_{\alpha0} &= \frac{N}{2} - \frac{1}{2}(2j_\alpha + 1).
\end{align*}
\]

(3.13)

Since the values for $N$ range from 0 to $2(2j_\alpha + 1)$ it
results that the minimum and maximum values of $J_{\alpha0}$ are $-(2j_\alpha + 1)/2$ and $(2j_\alpha + 1)/2$, respectively. Consequently, the quasispin has the expression:

\[
J_{\alpha} = \frac{1}{2}(2j_\alpha + 1).
\]

(3.14)

Thus, the state with a minimum quasispin projection to the $z$ axis is a kind of Hartree-Fock vacuum for the low-
ing 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 $j_\alpha$, while the quasispin is given by the semi-degeneracy of the given single particle state.

The transformation $\exp(-iF)$ 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 $\langle0|\exp(i\beta_{\alpha+}J_{\alpha-})$.

By means of Eqs. (2.20) and (2.21), we obtain

\[
\begin{align*}
\langle0| \exp(i\beta_{\alpha+}J_{\alpha-}) \exp(i\beta_{\alpha-}J_{\alpha+})|0\rangle = \\
= \langle0| \exp(-i\alpha_{\alpha-}J_{\alpha+}) \exp(-i\alpha_{\alpha+}J_{\alpha-})|0\rangle \\
= \langle0| \exp(-i\alpha_{\alpha0}J_{\alpha0})|0\rangle = \langle0| \exp(i\alpha_{\alpha0}(j_\alpha + \frac{1}{2}))|0\rangle \\
= \left(1 + \frac{1}{2}\beta_{\alpha+}\beta_{\alpha-}\right)^{2j_\alpha+1}.
\end{align*}
\]

(3.15)

In the above case, the parameter $\beta_{\alpha0}$ is equal to zero; we used Eq. (2.21) to express $\alpha_{\alpha0}$ in terms of $\beta_{\alpha+}$ and $\beta_{\alpha-}$.

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

\[
e^{-iF}J_{\mu\alpha}e^{iF} = \tilde{J}_{\mu\alpha}, \quad \mu = \pm, 0,
\]

where

\[
\begin{align*}
\tilde{J}_{\alpha+} &= -\frac{1}{\sqrt{2}} \sum_m c_{am}^\dagger d_{am}, \\
\tilde{J}_{\alpha-} &= -\frac{1}{\sqrt{2}} \sum_m c_{am} d_{am}, \\
\tilde{J}_{\alpha0} &= \frac{1}{2} \sum_m (c_{am}^\dagger c_{am} - d_{am}^\dagger d_{am}).
\end{align*}
\]

(3.16)
Under the action of a unitary BV transformation, the operator $e^{-iF}$ maps onto itself, since
\[
\tilde{\gamma} = e^{-iF}Fe^{iF} = \sqrt{2} \sum_{\alpha} \left( z_{\alpha} \sum_{m} c_{\alpha m}^{\dagger} d_{\alpha m} + z_{\alpha}^{*} \sum_{m} d_{\alpha m} c_{\alpha m} \right) = F.
\]
(3.17)

The reciprocal relation for Eq. (3.3) takes the form
\[
c_{\alpha m}^{\dagger} = e^{i\tilde{\gamma}} c_{\alpha m}^{\dagger} e^{-i\tilde{\gamma}},
d_{\alpha m}^{\dagger} = e^{i\tilde{\gamma}} d_{\alpha m}^{\dagger} e^{-i\tilde{\gamma}}
\]
or, explicitly,
\[
c_{\alpha m}^{\dagger} = U_{\alpha} c_{\alpha m}^{\dagger} + V_{\alpha} d_{\alpha m}^{\dagger},
d_{\alpha m}^{\dagger} = U_{\alpha} d_{\alpha m}^{\dagger} + V_{\alpha} c_{\alpha m}^{\dagger}.
\]
(3.18)

IV. PARTICLE NUMBER PROJECTION

The projection operator to the state with a definite number of particles is given by
\[
P_{N} = \int_{0}^{2\pi} \frac{d\varphi}{2\pi} e^{i(N-N)\varphi}.
\]
(4.1)

One can check that the signature property of a projection operator is satisfied:
\[
P_{N}P_{N} = P_{N}.
\]
(4.2)

The particle number operator can be expressed in terms of the operators $J_{\alpha0}$
\[
\hat{N} = \sum_{\alpha} \hat{N}_{\alpha},
\]
where
\[
\hat{N}_{\alpha} = 2J_{\alpha0} + 2J_{\alpha} + 1.
\]
(4.3)

The operator $P_{N}$ acting on the BCS wave function gives a state with a definite number of particles
\[
|BCS, N\rangle \equiv C_{N} P_{N} |BCS\rangle
\]
\[
= C_{N} \int_{0}^{2\pi} \frac{d\varphi}{2\pi} e^{i(N-N)\varphi} e^{-iF} |0\rangle
\]
\[
= C_{N} \int_{0}^{2\pi} \frac{d\varphi}{2\pi} e^{-iN\varphi} e^{-iF(\varphi)} |0\rangle,
\]
(4.4)

where
\[
F(\varphi) = - \sum_{\alpha} \left( z_{\alpha} e^{2i\varphi} J_{\alpha+} - z_{\alpha}^{*} e^{-2i\varphi} J_{\alpha-} \right)
\]
and $F = F(0)$.

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 $J_{\alpha}$:
\[
F(\varphi) = - \sum_{\alpha} \rho_{\alpha} (n_{\alpha-} J_{\alpha+} + n_{\alpha+} J_{\alpha-}).
\]
(4.6)

Here, $\mathbf{n}_{\alpha}$ are unit vectors defined by the cyclic coordinates
\[
n_{\alpha\pm} = \frac{1}{\sqrt{2}} \exp(\pm i(\psi_{\alpha} - 2\varphi)),
n_{\alpha0} = 0.
\]
(4.7)

Using Eq. (4.2), we obtain
\[
\exp(-iF(\varphi)) = \exp(i \sum_{\alpha} \rho_{\alpha} (n_{\alpha-} J_{\alpha+} + n_{\alpha+} J_{\alpha-}))
\]
\[
= \exp(i \sum_{\alpha} \alpha_{\alpha-} J_{\alpha+}) \times \exp(-i \sum_{\alpha} \alpha_{\alpha0} J_{\alpha0}) \exp(i \sum_{\alpha} \alpha_{\alpha+} J_{\alpha-}),
\]
where, according to Eqs. (2.12) and (2.13),
\[
\alpha_{\alpha\pm} = n_{\alpha\pm} 2 \tan(\rho_{\alpha}/2),
\]
\[
\alpha_{\alpha0} = -2i \ln(\cos(\rho_{\alpha}/2)).
\]
(4.8)

Acting with the operator $\exp(-iF(\varphi))$, after the factorizing it, on the vacuum state, we obtain
\[
\exp(-iF(\varphi))|0\rangle = \prod_{\alpha} \left( \cos^{2}(\rho_{\alpha}/2) \right)^{n_{\alpha}+1/2}
\]
\[
\times \exp(i \sum_{\beta} n_{\beta-} 2 \tan(\rho_{\beta}/2) J_{\beta+})|0\rangle.
\]

Now, we are in a position to find the projected state with $N$ nucleons.
The contour $C$ encompasses the point $\zeta = 0$, 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:

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

$$= C_N^2 \int_C \frac{d\zeta}{2\pi i} \frac{1}{\zeta^{N+1}} \prod_\alpha (\cos^2(\rho_\alpha/2) + \zeta^2 \sin^2(\rho_\alpha/2))^{2J_\alpha + 1}. \tag{4.9}$$

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 the Eqs. (2.20) and (2.21), which allow 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 to 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 $\alpha' = \alpha''$, i.e. 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

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

where

$$G_\beta(\zeta) = \sum_\alpha \left( \frac{\Omega_\beta}{N} \frac{\zeta^2 \sin^2(\rho_\beta/2)}{\cos^2(\rho_\beta/2) + \zeta^2 \sin^2(\rho_\beta/2)} \times \prod_\alpha (\cos^2(\rho_\alpha/2) + \zeta^2 \sin^2(\rho_\alpha/2))^{2J_\alpha + 1} \right), \tag{4.13}$$

with $\Omega_\beta = 2(2j_\beta + 1)$. We expand further the expression in front of the product sign in powers of $\zeta^2$. 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

$$Q(0) = \prod_{\alpha} (\cos^2(\rho_\alpha/2))^{2J_\alpha+1}. \quad (4.14)$$

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

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

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

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 difficulties. We avoid this difficulty by reducing the problem to the computation of the recursion relations. Within a variation after projection procedure the angles $\rho_\beta$ 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 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

$$\Omega = \sum_{\beta} \Omega_\beta. \quad (4.17)$$

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

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

These expressions should be supplemented by the boundary condition

$$Q(\Omega) = \prod_{\alpha} (\sin^2(\rho_\alpha/2))^{2J_\alpha+1}. \quad (4.19)$$

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

The only singularity of the integrand in the expression $Q(\Omega)$ 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 $1/\zeta$ is valid. Obviously, the results $Q(\Omega)$ and $Q(\Omega)$ coincide. Also we note that for $N = 0$ the function $Q^\beta(N)$ given by Eq. (4.19) is not defined. For this case one should use the $1/\zeta$ expansion from Eq. (4.19). By contrast for calculating $Q^\beta(\Omega)$ the expression $Q(\Omega)$ is the appropriate one. From the integral representation of $Q(N)$ as well as from Eq. (A.11) considered for the diagonal case, a very simple relation follows:

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

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

The average values of any fermion operator corresponding to the particle number projected BCS state, can be expressed in terms of the function $Q(N)$, which is the inverse of the normalization constant squared. In next Section this will be shown for 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 two body interaction whit a strength depending on shells

$$\tilde{H} = \sum_{\alpha} (\epsilon_\alpha - \lambda)N_\alpha + \sum_{\alpha\beta} V_{\alpha\beta}J_{\alpha+}J_{\beta-}. \quad (5.1)$$

Within the standard BCS formalism, $\lambda$ 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 $V_{\alpha\beta} = -2G$ 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 beta Fermi-type decay. Note that such a particular form of the $pn$ pairing interaction is not invariant under the rotations in the 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 $\tilde{H}$ 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.

\[ \langle N_\alpha \rangle = \langle BCS, N | N_\alpha | BCS, N \rangle. \]  

(5.2)

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

\[ \langle N_\alpha \rangle = Q^{-1}(N) \int_C \frac{d\zeta}{2\pi i} \mathcal{P}_\alpha(\zeta). \]  

(5.3)

where

\[ \mathcal{P}_\alpha(\zeta) = 2i \prod_\gamma (\cos^2(\rho_\gamma / 2))^{2j_\gamma + 1} \]

\[ \times \frac{d}{dx}(0) \exp(i \sum_\gamma \exp(i\psi_\gamma)\sqrt{2}\tan(\rho_\gamma / 2)J_{\gamma-}) \]

\[ \times \exp(-ix(J_{00} + j_\alpha + 1 / 2)) \]

\[ \times \exp(i\zeta^2 \sum_\gamma \exp(-i\psi_\gamma)\sqrt{2}\tan(\rho_\gamma / 2)J_{\gamma+}) \bigg|_{x=0}. \]

The derivative over \( x \) is taken at \( x = 0 \). Making use of Eqs. 2.2, 2.20 and 2.21, \( \mathcal{P}_\alpha(\zeta) \) can be simplified to give:

\[ \mathcal{P}_\alpha(\zeta) = N\mathcal{G}_\alpha(\zeta). \]  

(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

\[ \langle N_\alpha \rangle = NQ^\alpha(N)Q^{-1}(N). \]  

(5.6)

The sum over \( \alpha \) in Eq. 5.6 gives identity \( N = N \). Using Eq. 4.3, one can find the average of \( J_{00} \).

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

\[ \langle J_{\alpha+} \rangle = \langle BCS, N + 2 | J_{\alpha+} | BCS, N \rangle \]

\[ = C_{N+2}(BCS) | J_{\alpha+} | BCS, N \rangle. \]  

(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 Appendix A. Here, following the path described in the previous subsection, we present results for the matrix elements diagonal in the BCS angles:

\[ \langle J_{\alpha+} \rangle = -iQ^{-1/2}(N + 2)Q^{-1/2}(N) \frac{1}{2\sqrt{2}} \]

\[ \times \exp(i\psi_\alpha)\cot(\rho_\alpha / 2)Q^\alpha(N + 2). \]  

(5.8)

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

\[ \langle J_{\alpha+} \rangle = iQ^{-1/2}(N + 2)Q^{-1/2}(N)(2j_\alpha + 1) \frac{1}{2\sqrt{2}} \]

\[ \times \exp(-i\psi_\alpha) \sum_{n=0}^N (-1)^n\tan^{2n+1}(\rho_\alpha / 2)Q(N - 2n). \]  

(5.9)

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

\[ \langle J_{\alpha-} \rangle = \langle BCS, N | J_{\alpha-} | BCS, N + 2 \rangle \]

\[ = -\langle J_{\alpha+} \rangle^*. \]  

(5.10)

This quantity multiplied by \( \sqrt{2} \) defines the spectroscopic factor for a pair \( \alpha \) of states which could be measured in a deuteron transfer reaction. If the two body interaction strength is state independent and equal to \( -G/4 \) the pairing interaction term resembles the pairing interaction for alike nucleons. In virtue of the particle number conservation, the average of \( G\sqrt{2} \sum_\alpha J_{\alpha+} \) is equal to zero. By analogy with the case of alike nucleon pairing, we call the sum

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

(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 \( \langle pn \rangle \) pairing interaction with the generic term:

\[ \langle J_{\alpha+} J_{\beta-} \rangle = \langle BCS, N | J_{\alpha+} J_{\beta-} | BCS, N \rangle. \]  

(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 in origin:

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

(5.13)
where
\[
P_{\alpha\beta}(\zeta) = -\prod_{\gamma}(\cos^2(\rho_\gamma/2))^{2j_\gamma+1}
\] (5.13)
\[
\times \frac{d}{dx} \frac{d}{dy} (0) \exp\left(i \sum_{\gamma} \exp(i\psi_\gamma) \sqrt{2} \tan(\rho_\gamma/2) J_{\gamma-}\right)
\times \exp(-ixJ_{\alpha+}) \exp(-iyJ_{\beta-})
\times \exp(i\zeta^2 \sum_{\delta} \exp(-i\psi_{\delta}) \sqrt{2} \tan(\rho_\delta/2) J_{\delta+}|0\rangle |_{x=y=0}.
\]

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

The final expressions for $\alpha \neq \beta$ and $\alpha = \beta$ become
\[
\langle J_{\alpha+}J_{\beta-} \rangle = Q^{-1}(N) \frac{1}{4} N(2j_\beta + 1)Q^\alpha(N) - (2j_\alpha + 1)Q^\beta(N) \exp(i\psi_\beta - i\psi_\alpha) \tan(\rho_\beta/2) \tan(\rho_\alpha/2) \tan^2(\rho_\beta/2) - \tan^2(\rho_\alpha/2),
\] (5.14)
\[
\langle J_{\alpha+}J_{\alpha-} \rangle = -Q^{-1}(N) \frac{N}{2} Q^\alpha(N) + (j_\alpha + 1/2) \sum_{n=1}^{N/2} (-)^{n+1} \tan^2(\rho_\alpha/2)(2nj_\alpha - 1)Q(N - 2n).
\] (5.15)

After some algebraic manipulations one finds a Bernoulli distribution
\[
Q(N) = \left( \frac{2j_\alpha + 1}{N/2} \right) p^{N/2}(1 - p)^{2j_\alpha + 1 - N/2}
\] (6.2)
with probability $p = \sin^2(\rho/2)$, that can be written, in fact, immediately starting from the integral form
\[
\int \frac{1}{N!} \frac{1}{M!} \left( \frac{1}{2} \right)^{N+M} (2\pi)^2 \sum_{\alpha,\beta,\gamma,\delta} \left| V_{\alpha\beta} \right|^2
\] (6.1)
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. (6.1), now has the form
\[
V_{\alpha\beta} = 2G.
\] (6.3)

The corresponding energies of the shells are denoted by $\epsilon_1$ and $\epsilon_2$, respectively.

### A. Standard BCS

If one neglect the renormalization of the single particle energies due to the pairing interaction, the energy of the constrained system of $N$ nucleons has the expression:
\[
E'(N) = \sum_{\alpha} 2(2j_\alpha + 1)(\epsilon_\alpha - \lambda)|V_\alpha|^2 - \frac{\Delta^2}{G},
\] (6.4)
with
\[
\Delta = G \sum_{\alpha} 2(2j_\alpha + 1)U_\alpha V_\alpha, \quad N = \sum_{\alpha} 2(2j_\alpha + 1)|V_\alpha|^2.
\] (6.5)
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 $\Delta$ and the parameter $\lambda$:

\[
\left( \frac{|V_\alpha|^2}{U_\alpha^2} \right) = \frac{1}{2} \left( 1 + \frac{\epsilon_\alpha - \lambda}{\sqrt{(\epsilon_\alpha - \lambda)^2 + |\Delta|^2}} \right).
\]

The energy gap and $\lambda$ can be found from the self-consistency condition (6.3) and the particle number constraint (6.4):

\[
\sum_\alpha \frac{(2j_\alpha + 1)(\epsilon_\alpha - \lambda)}{\sqrt{(\epsilon_\alpha - \lambda)^2 + |\Delta|^2}} = \sum_\alpha (2j_\alpha + 1) - N,
\]

\[
\frac{G}{2} \sum_\alpha \frac{2j_\alpha + 1}{\sqrt{(\epsilon_\alpha - \lambda)^2 + |\Delta|^2}} = 1.
\]

The variational problem also constrains the phases. Denoting by $\varphi$ the phase of the gap parameter

\[
\Delta = |\Delta|e^{i\varphi},
\]

one successively find $\arg V_\alpha = \arg \Delta$ or, using the relation (6.7),

\[
\psi_\alpha + \frac{\pi}{2} = \varphi.
\]

The average energy (6.4) is independent of the phase factor of $V_\alpha$. 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. (6.14).

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

\[
\epsilon_1 - \lambda = \frac{1}{2} G(2j + 1 - N),
\]

\[
\Delta^2 = \frac{1}{4} G^2 N(4j + 2 - N),
\]

\[
V_j^2 = \frac{N}{2(2j + 1)},
\]

\[
E'(N) = -\frac{G}{4} N^2.
\]

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:

\[
E_{gs}(N) = \epsilon_1 N - \frac{1}{4} GN(4j + 2 - N).
\]

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 of is independent of the BCS angles and phases, and equal to

\[
E(N) = \epsilon_1 N - \frac{1}{4} GN(4j + 4 - N).
\]

This result can be obtained with the general formulas of the previous Sections, where $\lambda$ is set equal to zero but also by exploiting the fact that after projecting the nucleon total number, in the BCS wave function survives only the component $\sim (J_+)^{N/2}(0)$. The average value of the Hamiltonian $\tilde{H}$, 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.

Moreover 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 quasi-rotation group, $J_\alpha^2$, and the quasi-spin projection on z-axis, $J_\alpha^0$. 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 shells calculations. For what follows it is useful to write the expression of the Q function in a more compact form. The reciprocal norm squared can be written as:

\[
Q(2) = T_2 Q(0), \quad Q(4) = \frac{1}{2} (T_2^2 - T_4) Q(0), \quad Q(6) = \frac{1}{6} (T_2^3 - 3T_2 T_4 + 2T_6) Q(0),
\]

\[
Q(8) = \frac{1}{24} (T_2^4 - 6T_2^2 T_4 + 8T_2 T_6 + 3T_4^2 - 6T_6) Q(0), \quad Q(10) = \frac{1}{5} \sum_{k=1}^5 T_{2k} Q(10 - 2k)
\]

where

\[
Q(0) = (\cos^2(\rho_1/2))^2 + (\cos^2(\rho_2/2))^2 + 1,
\]

\[
T_n = (2j_1 + 1) \tan^n(\rho_1/2) + (2j_2 + 1) \tan^n(\rho_2/2).
\]

The terms $Q^n(N)$ specified by (4.16) acquire also compact forms:

\[
Q^n(2) = F_{n2} Q(0), \quad Q^n(4) = \frac{1}{2} Q(0) (T_2 F_{n2} - F_{n4}),
\]

\[
Q^n(6) = \frac{1}{3} Q(0) \left( \frac{1}{2} (T_2^2 - T_4) F_{n2} - T_2 F_{n4} + F_{n6} \right), \quad Q^n(8) = \frac{1}{6} Q(0) \left( \frac{1}{2} (T_2^3 - 3T_2 T_4 + 2T_6) F_{n2}
\]

\[- \frac{1}{2} (T_2^2 - T_4) F_{n4} + T_2 F_{n6} - F_{n8} \right), \quad Q^n(10) = \sum_{p=1}^5 F_{n,2p} (-1)^{p+1} Q(10 - 2p).
\]
FIG. 1: The energy of a system with N nucleons ($N = 2, 4, 6, 8$), obtained within the BCS formalism, is plotted as function of the pairing interaction strength, $G$.

\[
\begin{array}{|c|c|c|c|}
\hline
\text{G=0.1 MeV} & \text{G=1.0 MeV} \\
\hline
\text{N=2} & \text{N=8} & \text{N=2} & \text{N=8} \\
\hline
E_{\text{BCS}} & 1.37573 & -8.35069 & 6.93772 & -21.38316 \\
\Delta & 0.30183 & 3.31395 & 0.51425 & 5.65241 \\
E_{\text{PBCS}} & 1.25987 & -9.35235 & 6.48216 & -25.38779 \\
E_{\text{FBCS}} & 1.25969 & -9.35235 & 6.48213 & -25.38779 \\
\Delta^{(N)} & 0.4292 & 4.6866 & 0.5753 & 6.3196 \\
\hline
\end{array}
\]

TABLE I: The ground state energy provided by the BCS, PBCS and FBCS formalism, respectively, given in MeV, are listed for two values of the nucleon total number and two values of the pairing strength, $G$.

where

\[
F_{\alpha n} = (2j_\alpha + 1) \tan^n(\rho_\alpha/2).
\]

Using these partial results in connection with 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 projection after variation approach, PBCS, and the projection before variation formalism, FBCS. Also, the exact eigenvalues of $\hat{H}$ have been obtained by diagonalization. The input data in our calculation are:

FIG. 2: The energy of a system with N nucleons ($N = 2, 4, 6, 8$), obtained within the PBCS formalism, is plotted as 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, Exact.

FIG. 3: The gap energy for a system with N nucleons ($N = 2, 4, 6, 8$) is plotted as function of the pairing interaction strength, $G$, within the standard BCS formalism.
Results for energies are plotted, in Fig. 1, as function of $(6.8)$ and then calculated the ground state energy $(6.4)$. We conventionally call this approach as projected BCS for a given by the present formalism with the energy was calculated with the general expression provided by the standard BCS approach, the system energy was calculated with the normal expression provided by Eq. (5.11).

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

$$E_{normal} = N \epsilon_1.$$  \hspace{1cm} (6.18)

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 call this approach as 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 others 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 particle total 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. To get a better view on the quantitative energy split due to its $N$-dependence we collected the energy values for the extreme values of $N$, in Table I. From there one can see that the energy ordering for a given $G$ is not depending on $N$. Indeed, for $G = 0.1$ MeV the ordering for $N = 2$ and $N = 8$ are:

$$E_{normal} > E_{BCS} > E_{PBCS} > E_{FBCS}, \ N = 2, 8,$$

while for $G = 1.0$ MeV the energy order is as:

$$E_{normal} > E_{BCS} > E_{PBCS} = E_{FBCS}, \ N = 2, 8.$$

It is remarkable the fact that energies provided by the PBCS and FBCS approaches are practically the same. Only very tiny differences are noticed for $G=0.1$ MeV, which might be caused by the numerical procedures adopted for the two cases.

Due to the above mentioned ordering for the ground state energies provided by different formalism we may conclude that for all cases the superconducting phase is achieved for any $G \geq 0.1$. Another observable considered in our study is the energy gap obtained within the standard BCS and the FBCS formalism, respectively. The results obtained for a fixed $N$ were plotted as function of $G$ in figure 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 $\Delta$ than for $\Delta^{(N)}$. Indeed, according to the data listed in Table I, $\Delta(N = 8) - \Delta(N = 2)$ is equal to 0.212 MeV and 2.338 MeV for $G$ equal to 0.1 MeV and 1.0 MeV respectively, while $\Delta^{(8)} - \Delta^{(2)}$ for $G = 0.1; 1.0$ MeV, amounts to 0.146 MeV 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, $N$

$$|N_1, N_2\rangle = C_{N_1 N_2} (c_{1d}^\dagger)^{N_1/2} (c_{2d}^\dagger)^{N_2/2} |0\rangle,$$

$$N_1 + N_2 = N.$$  \hspace{1cm} (6.19)

with $C_{N_1 N_2}$ standing for the normalization constant. The matrix elements of $\hat{H}$ in this basis have simple expressions:
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 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.

VII. CONCLUSIONS

Many interesting properties of the $pn$ pairing have been derived using for the BCS function the form (3.1). After making use of the factorization described in Section I, one finds out that the function (3.1) for a fixed $\alpha$ 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 this equation the norm of a projected state with $N$ particles is related with the norms of the $N'$-projected states with $N' < N$. For pairing interaction of alike nucleons, a similar recursion formula was obtained in Ref. (6). The difference between the two recursion formulas consists of that there the recursion is operating in two dimensions, there are two indices which 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 spectroscopic factor for a deuteron transfer reaction. Being guided by the analogy with the alike 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 Appendix A the matrix element involved in the width of an $\alpha$ 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 beta 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 function of the particle number $N$ and the parameters $\rho_\alpha, \psi_\alpha$ 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 to 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 both in the standard BCS and projected BCS formalism. 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, 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 be however improved by adding to (3.1) two factors accounting for the proton-proton and neutron-neutron pairing, respectively.

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 the proton-neutron $T=0$ pairing as well as the 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.

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Appendix A: 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 Section V. Here we derive formulas for \( \langle BCS_f, N | BCS_i, N \rangle \) for \( O = 1, J_{\pm \alpha}, J_{\pm \alpha} J_{\pm \beta} \) and \( J_{\pm \alpha} J_{\pm \beta} \) with different BCS angles of the final and initial states.

We start from the diagonal in particle number overlap

\[
\langle BCS_f, N | BCS_i, N \rangle = Q_f^{-1/2}(N) Q_i^{-1/2}(N) Q_{fi}(N),
\]

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 Section V give give the off-diagonal \( Q \)-function

\[
Q_{fi}(N) = \int \frac{d \zeta}{2 \pi i} \frac{1}{\zeta^{N+1} + \zeta^{N-1}} \prod_\alpha (\cos(\rho'_\alpha/2) \cos(\rho_\alpha/2) + \zeta^2 \exp(i \psi'_\alpha - i \psi_\alpha) \sin(\rho'_\alpha/2) \sin(\rho_\alpha/2))^{2j_\alpha + 1}.
\]  

(A.1)

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

\[
Q_{fi}(N) = \sum_\alpha Q_{fi}^\alpha(N),
\]

\[
Q_{fi}^\alpha(N) = \frac{\Omega_\alpha}{N} \sum_{n=1}^{N/2} (-)^{n+1} (\exp(i \psi'_\alpha - i \psi_\alpha) \tan(\rho'_\alpha/2) \tan(\rho_\alpha/2))^n Q_{fi}(N - 2n)
\]

(A.2)

\[= \frac{\Omega_\alpha}{\Omega - N} \sum_{n=1}^{(\Omega - N)/2} (-)^{n+1} (\exp(-i \psi'_\alpha + i \psi_\alpha) \cot(\rho'_\alpha/2) \cot(\rho_\alpha/2))^n Q_{fi}(N + 2n).\]  

(A.3)

The boundary conditions follow from (A.1)

\[
Q_{fi}(0) = \prod_\alpha (\cos(\rho'_\alpha/2) \cos(\rho_\alpha/2))^{2j_\alpha + 1},
\]

\[
Q_{fi}(\Omega) = \prod_\alpha (\exp(i \psi'_\alpha - i \psi_\alpha) \sin(\rho'_\alpha/2) \sin(\rho_\alpha/2))^{2j_\alpha + 1}.
\]

As in the case of the function \( Q(N) \), \( Q_{fi}(N) \) 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, \( Q_f(N) = Q_f(N) \) and \( Q_{i\alpha}(N) = Q_{i\alpha}(N) \). \( Q_{fi}^\alpha(N) \) vanishes outside the interval \((2, \Omega - 2)\).

Now, consider the 2-fermion gap function

\[
\langle J_{\alpha+} \rangle_{fi} = \langle BCS_f, N + 2 | J_{\alpha+} | BCS_i, N \rangle
\]

\[= Q_f^{-1/2}(N + 2) Q_i^{-1/2}(N) \left\langle \frac{N}{2} Q_{fi}^\alpha(N) - (j_\alpha + 1/2) Q_{fi}(N) \right\rangle.
\]  

(A.4)

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

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

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

\[
\langle J_{\alpha+} \rangle_{fi} = -i Q_f^{-1/2}(N + 2) Q_i^{-1/2}(N) \frac{1}{2\sqrt{2}} (N + 2) \exp(i \psi_\alpha) \cot(\rho_\alpha/2) Q_{fi}^\alpha(N + 2),
\]

\[
\langle J_{\alpha0} \rangle_{fi} = Q_f^{-1/2}(N) Q_i^{-1/2}(N) \left( \frac{N}{2} Q_{fi}^\alpha(N) - (j_\alpha + 1/2) Q_{fi}(N) \right).
\]  

(A.5)

Summing the last equation over \( \alpha \) one arrives at:

\[
2 \sum_\alpha \langle J_{\alpha0} \rangle_{fi} = Q_f^{-1/2}(N) Q_i^{-1/2}(N) Q_{fi}(N)(N - \frac{1}{2} \Omega),
\]

which is consistent with the definition for particles num-
The expression for \( \langle J_\alpha^- \rangle_{fi} \) is obtained by complex conjugation \( (A.3) \).

Consider now the 4-fermion gap function

\[
\langle J_\alpha^+ J_\beta^+ \rangle_{fi} = \langle BCS_f, N+4| J_{\alpha^+} J_{\beta^+} | BCS_i, N \rangle.
\]

This matrix element represents the width of the \( \alpha \) 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 these matrix elements one may define the spectroscopic factor of a reaction which removes an \( \alpha \) particle from the states \( \alpha \) and \( \beta \). In other words squaring this matrix element one obtains the occupation probabilities of the states \( \alpha \) and \( \beta \) 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 Section II. For \( \alpha \neq \beta \), we obtain

\[
\langle J_{\alpha^+} J_{\beta^+} \rangle_{fi} = -Q_f^{-1/2}(N+4)Q_i^{-1/2}(N) \frac{1}{4} (N+2)((2j_\beta + 1)Q_f^3(N + 2) - (2j_\alpha + 1)Q_i^3(N + 2))
\]

\[
\times \frac{\exp(i\psi_\beta + id_\alpha') \tan(\rho_\alpha'/2) \tan(\rho_\beta/2)}{\exp(i\psi_\alpha - i\psi_\alpha') \tan(\rho_\alpha'/2) \tan(\rho_\alpha/2) - \exp(i\psi_\beta' - i\psi_\beta) \tan(\rho_\beta/2) \tan(\rho_\beta/2)}.
\]

\[
(A.6)
\]

Similar expression is obtained for the matrix element

\[
\langle J_{\alpha^+} J_{\beta^-} \rangle_{fi} = \langle BCS_f, N| J_{\alpha^-} | BCS_i, N \rangle
\]

\[
= -Q_f^{-1/2}(N)Q_i^{-1/2}(N) \frac{1}{4} N((2j_\beta + 1)Q_f^3(N) - (2j_\alpha + 1)Q_i^3(N))
\]

\[
\times \frac{\exp(i\psi_\beta' - i\psi_\alpha') \tan(\rho_\beta/2) \tan(\rho_\alpha/2)}{\exp(i\psi_\alpha' - i\psi_\alpha) \tan(\rho_\alpha'/2) \tan(\rho_\alpha/2) - \exp(i\psi_\beta' - i\psi_\beta) \tan(\rho_\beta'/2) \tan(\rho_\beta/2)}.
\]

\[
(A.7)
\]

We may ask ourselves how this situation may appear? The answer is offered by the double beta decay with/without neutrinos in the final state. Indeed, in such a process the nucleus \( |N, Z \rangle \) goes to the nucleus \( |N-2, Z+2 \rangle \), two electrons and two/zero anti-neutrinos. 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 important in describing some important physical processes.

The average \( (A.6) \) is symmetric under interchange of the indices and \( \langle J_{\alpha^+} J_{\beta^-} \rangle_{fi} = \langle J_{\beta^-} J_{\alpha^+} \rangle_{fi} \). Complex conjugation of \( (A.6) \) allows to find \( \langle J_{\alpha^-} J_{\beta^-} \rangle_{fi} \).

When shells are the same, the result is as follows

\[
\langle J_{\alpha^+} J_{\alpha^+} \rangle_{fi} = -Q_f^{-1/2}(N+4)Q_i^{-1/2}(N) \frac{j_\alpha}{2} \exp(i\psi_\alpha + id_\alpha') \tan(\rho_\alpha'/2) \cot(\rho_\alpha/2)
\]

\[
\times \sum_{n=0}^{N/2} (-)^n (\exp(i\psi_\alpha' - i\psi_\alpha) \tan(\rho_\alpha'/2) \tan(\rho_\alpha/2))^n (N + 2 - 2n) Q_f^3(N + 2 - 2n) \tag{A.8}
\]

\[
= -Q_f^{-1/2}(N+4)Q_i^{-1/2}(N)j_\alpha(2j_\alpha + 1) \exp(2i\psi_\alpha') \tan^2(\rho_\alpha'/2)
\]

\[
\times \sum_{n=0}^{N/2} (-)^n (\exp(i\psi_\alpha' - i\psi_\alpha) \tan(\rho_\alpha'/2) \tan(\rho_\alpha/2))^n (n + 1) Q_f(N - 2n), \tag{A.9}
\]

\[
\langle J_{\alpha^-} J_{\alpha^-} \rangle_{fi} = -Q_f^{-1/2}(N)Q_i^{-1/2}(N) \frac{N}{2} Q_f^3(N)
\]

\[
+ (j_\alpha + 1/2) \sum_{n=1}^{N/2} (-)^{n+1} (\exp(i\psi_\alpha' - i\psi_\alpha) \tan(\rho_\alpha'/2) \tan(\rho_\alpha/2))^n (2nj_\alpha - 1) Q_f(N - 2n)). \tag{A.10}
\]

The representations \( (A.8) \) and \( (A.9) \) are equivalent.

The formalism allows also to provide an expression for the average as a sum over the quantum numbers \( \alpha \) for a fixed number of the particles as well. However, the number of shells is usually much larger than \( N \), and the ratio between \( \Omega \) and \( N \) indicates the accuracy of the so-
olution 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 therefore preferable. Also, the recursive computation of the function $Q_f(N)$ starting from small numbers of particles is more simple.

The function $Q_f(N)$ can be written in the form:

$$Q_f(N) = \sum_{N_1+N_2+\ldots=N} \prod_{\alpha} \frac{(\Omega_\alpha/2)!}{(\Omega_\alpha/2-N_\alpha/2)!(N_\alpha/2)!} \left(\exp(-i\psi'_\alpha + i\psi_\alpha)\sin(\rho'_\alpha/2)\sin(\rho_\alpha/2)\right)^{N_\alpha/2} \times \left(\cos(\rho'_\alpha/2)\cos(\rho_\alpha/2)\right)^{\Omega_\alpha/2-N_\alpha/2}.$$  \hspace{1cm} (A.11)

Here the summation is over all sets of occupation numbers $N_\alpha$, which gives the total number of particle $N$, the occupation numbers are even. In the special case of a single shell, we reproduce the equation [6.2].

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