Chapter 1

Pairing in finite systems: beyond the HFB theory

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The Hartree-Fock-Bogoliubov approximation is very useful for treating both long- and short-range correlations in finite quantum fermion systems, but it must be extended in order to describe detailed spectroscopic properties. One problem is the symmetry-breaking character of the HFB approximation. We present a general and systematic way to restore symmetries and to extend the configuration space using pfaffian formulas for the many-body matrix elements. The advantage of those formulas is that the sign of the matrix elements is unambiguously determined. It is also helpful to extend the space of configurations by constraining the HFB solutions in some way. A powerful method for finding these constrained solutions is the gradient method, based on the generalized Thouless transformation. The gradient method also preserves the number parity of the Bogoliubov transformation, which facilitates the application of the theory to systems with odd particle number.

1. Introduction

Soon after the seminal paper describing the microscopic theory of superconductivity by Bardeen-Cooper-Schrieffer (BCS) [1], Bohr et al. [2] found an analogy between the excitation spectra of nuclei and those of the superconducting metallic state and pointed out the role of pairing correlations in the low excitation spectrum of atomic nuclei. As self-bound fermionic systems, nuclei are unique in requiring for their theoretical description the inclusion of both long- and short-range correlations. The longest range correlations
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may be treated in the Hartree-Fock (HF) approximation with a suitable effective Hamiltonian. In the simplest theory that includes pairing, the pairing correlations are introduced through the BCS approximation defining the pair amplitudes from the time-reversed orbital wave functions of the HF theory. However, in many situations the HF/BCS wave functions are not the variational minima in the complete space of wave functions defined by the Bogoliubov transformations. For this reason contemporary calculations of nuclear structure based on the mean-field approximation (see [3–5] for recent reviews) largely follow the Hartree-Fock-Bogoliubov (HFB) formulation of theory; see Refs [6, 7] for details in the nuclear physics context.

The atomic nucleus is a mesoscopic system where the broken symmetry implied by the BCS or HFB wave functions is just an artifact of the mean field approximation. An improved description of physical properties requires techniques beyond the mean field, like particle number symmetry restoration or fluctuations in the BCS order parameter. Those techniques were developed in the 1960’s [8–11] and applied to a variety of situations in nuclear physics [3–5]. Recently, they have been exported to several branches of physics [12] and quantum chemistry [13]. Other approaches based on the Random Phase approximation and derivatives are also popular (see Y.R. Shimizu contribution to this Volume and Ref [14]). However, technical difficulties still remain in its practical implementation, especially in systems where time reversal symmetry is broken. One of the difficulties is evaluating the sign of matrix elements between two general HFB wave functions. The sign is relevant because it determines the interference pattern of those linear combinations of mean field wave functions typical of theories for symmetry restoration and/or configuration mixing. The proof that the sign of the matrix elements is well defined was given in the past [15] but a general and robust methodology to determine it in practice was not available until a new method based on pfaffians was introduced [16]. The generalization to systems with an odd number of particles (to be denoted odd-A systems) has been given recently [17] and our methodology will be discussed below.

The HFB theory defines a minimization problem that raises the practical question of finding the minimum of an energy function that depends on a large number of variables. Traditionally the equation for the gradient, i.e. the derivative of the energy function with respect to all the variables, is set equal to zero and the resulting HFB equations are solved iteratively. However, it has been long known that there can be severe difficulties with this approach, as may be seen in Fig 5.3 of the textbook by Ring and Schuck [6]. The approach using the gradient directly is more stable, and
we have taken this path in our group at Madrid to develop efficient codes based on a second-order treatment of the gradient. One situation where the gradient method has obvious advantages is in treating systems with an odd number of particles, discussed in Section 3 below. It is also much easier to treat a large number of constraints in the gradient method. This will facilitate the extensions of the HFB theory discussed in Section 2 below.

2. Sign of HFB overlaps with the pfaffian technique

The problem of calculating the overlap of two HFB wave functions was first considered in the 1960’s [10] in the context of symmetry restoration. The formula derived there involves the square root of the determinant of a matrix built with the Bogoliubov amplitudes $U$ and $V$ of the HFB states involved. The presence of the square root implies that the sign is undefined. However, if time reversal is preserved, Kramers degeneracy implies that the determinant in the overlap formula is the square of a number and its sign is usually assigned to the overlap (without proof). For general HFB states it can be proven [15] that the eigenvalues of the matrix in the argument of the determinant are doubly degenerate implying that the determinant is again the square of a number.

![Fig. 1. Sketch of the real and imaginary parts of a typical overlap of the form $\langle w | \hat{R}_z (\alpha) | w' \rangle$. Filled circles are the values of the overlap; open circles the same but with the opposite sign.](image)

To illustrate the sign problem we present in Fig 2 a sketch of the real
and imaginary parts of a typical overlap of the form $\langle w|\hat{R}_z(\alpha)|w'\rangle$ where the angle $\alpha$ varies between 0 and $2\pi$. Realistic examples are presented and discussed, for instance, in Ref [18]. In our sketch plot, two sets of points are depicted. The filled circles represent the overlaps obtained on a discrete mesh of $\alpha$ values. The open circles are the same overlaps but with opposite sign. The lines joining the points are plotted to guide the eye. The overlaps are used typically in integrals in $\alpha$ (see [19] for examples). From the plot it becomes clear that if the procedure to identify the sign is not robust (usually arguments based on continuity of the overlap as a function of $\alpha$ are used) one can easily jump onto the wrong curve when the modulus of the overlap is small. At first sight it could be argued that the error in the integral is going to be small as the jump takes place in the region of small overlap moduli but continuing in the wrong curve leads to large values of the overlaps with the wrong sign.

An unambiguous evaluation of the sign of the overlap between two HFB wave functions was first achieved in Ref [16]. That expression for the overlap was derived by the coherent fermion state technique, resulting in a pfaffian of a matrix related to the Bogoliubov transformation matrices. While this solves the problem for fully paired HFB wave functions, the matrix expression can become singular in the HF limit. Other pfaffian expressions addressing this and other problems related with the use of different finite bases for different states were subsequently found [20]. The limitation in these approaches is that only fully paired HFB wave functions are allowed and the method is restricted to systems with even number parity. Recently, a method that uses the expression of the standard Wick theorem for mean values of fermion operators in the vacuum in terms of a pfaffian has permitted the extension of the previous result to odd-A systems [17]. Other treatments of odd-A systems [18, 21] require the Generalized Wick Theorem (GWT) [11] and lead to more elaborated expressions.

The results obtained in [17] are based on a result for the expectation values of fermion operators in the vacuum. The method may be understood more easily with an example. If $\beta_i$ are fermion creation or annihilation operators satisfying the standard commutation relations, the standard Wick theorem says that the following mean value with respect to the vacuum

$$\langle -|\beta_1\beta_2\beta_3\beta_4|-\rangle = r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$$

is given in terms of the contractions $r_{ij} = \langle -|\beta_i\beta_j|-\rangle$. On the other hand,
the Pfaffian of a general $4 \times 4$ (skew-symmetric) matrix is given by

\[
\text{pf}
\begin{pmatrix}
0 & r_{12} & r_{13} & r_{14} \\
-r_{12} & 0 & r_{23} & r_{24} \\
-r_{13} & -r_{23} & 0 & r_{34} \\
-r_{14} & -r_{24} & -r_{34} & 0
\end{pmatrix}
= r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}.
\]

This is exactly the same expression obtained for the above expectation value. This suggests the following result:

\[
\langle | \beta_1 \ldots \beta_P \bar{\beta}_1 \ldots \bar{\beta}_Q | \rangle = \text{pf}(S_{ij})
\tag{1}
\]

where $S_{ij}$ is the skew symmetric $(P + Q) \times (P + Q)$ matrix such that $S_{ij}$ $i < j$ are all the possible contractions

\[
\langle | \beta_k \bar{\beta}_l | \rangle \quad i, j = 1, \ldots, P(k, l = 1, \ldots, P)
\tag{2}
\]

\[
\langle | \beta_k \bar{\beta}_r | \rangle \quad i = 1, \ldots, P, j = P + 1, \ldots, P + Q(k = 1, \ldots, P; r = 1, \ldots, Q)
\tag{3}
\]

\[
\langle | \bar{\beta}_r \bar{\beta}_s | \rangle \quad i, j = P + 1, \ldots, P + Q(r, s = 1, \ldots, Q)
\tag{4}
\]

We have also introduced another set of fermion operators $\bar{\beta}_i$ that are presumably related to the $\beta_i$ by some canonical transformation. The proof of this result can be easily obtained using recursion relations and can also be easily extended to finite temperature systems \[23\].

The formula Eq. (1) can be readily applied to the problem of computing overlaps between two HFB wave functions by noting that such HFB states can be written as

\[
|w\rangle = \frac{\det C}{\prod_{\alpha=1}^n v_\alpha} \beta_1 \beta_2 \ldots \beta_{2n}|\rangle
\tag{5}
\]

where the normalization factor in front of the product of quasiparticle annihilation operators $\beta_i$ contains the occupancies $v_\alpha$ and the determinant of the third transformation in the Bloch-Messiah theorem \[6, 7\] and is constructed to give a normalized $|w\rangle$. An immediate application of this result is the formula for the overlap of two HFB states including a canonical transformation operator $\mathcal{R}$ (as the ones that appear when symmetry operations are applied to the system) acting on one of the states

\[
\langle w | \mathcal{R} | w' \rangle = (-1)^n \frac{\det C^* \det C'}{\prod_{\alpha=1}^n v_\alpha v'_\alpha} \text{pf}
\begin{pmatrix}
V^T U & V^T R V^{t*} \\
-V^t R V & U^t V^{t*}
\end{pmatrix}
\tag{6}
\]

See \[18\] for basic results and bibliography concerning Pfaffians and \[22\] for numerical and symbolic techniques.
where the matrix $R$ is the representation of the canonical transformation operator $\mathcal{R}$ on the linear Fock space generated by the creation and annihilation operator $c_i^\dagger$ and $c_i$ in some convenient basis, namely $\mathcal{R}c_i^\dagger\mathcal{R}^{-1} = \sum_j R_{ij}c_j^\dagger$.

A general multi-quasiparticle overlap including a canonical transformation $\mathcal{R}$ is easily obtained with the previous formalism \cite{17}:

$$\langle w|\bar{\beta}_{\mu r}\cdots \bar{\beta}_{\mu 1} R \bar{\beta}_{\nu s}^\dagger \cdots \bar{\beta}_{\nu 1}^\dagger|w'\rangle = (-1)^n (-1)^{(r-1)/2} \frac{\det C^* \det C'}{\prod_{\alpha \nu} \det \gamma_{\alpha \nu}} \times (7)$$

For this expression to make sense both $r$ and $s$ must have the same number parity. The objects $p$ and $q$ ($p'$ and $q'$) are matrices of dimension $r \times 2n$ ($s \times 2n$) with matrix elements $p_{\mu j} = \bar{V}_{\mu j}$ and $q_{\mu j} = \bar{U}_{\mu j}$. This expression has the advantage over the direct application of the generalized Wick’s theorem \cite{11} that it avoids the combinatorial explosion of terms to be evaluated. Namely, $(r + s - 1)!$ contractions have to be computed if the multi-quasiparticle overlap is evaluated by the generalized Wick’s theorem. To give an idea of the complexity brought about by the combinatorial explosion, let us just mention, for instance, that in the evaluation of the Hamiltonian overlap of two quasiparticle excitations built on top of an odd-A system, overlaps with ten quasiparticles are required. The number of terms to be considered if using the GWT would be $9!! = 945$. If two independent two quasiparticle excitations are considered in each isospin channel the number of quasiparticle operators increases by four and the number of contractions goes up to a whooping $13!! = 135 135$.

3. Gradient method for the HFB equation of odd-A systems

Systems with an odd number of particles are less studied from a theoretical perspective than even-even systems. Several circumstances could explain this imbalance and we now discuss two of them. At the BCS level the wave function of an odd-A system is given by \cite{6,7}

$$|\phi_{k_0}\rangle = a_{k_0}^+ \prod_{l \neq k_0} (u_l + v_l a_l^+ a_l^\dagger)|-\rangle$$

where the orbital labeled $k_0$ is “blocked”. As a consequence, this orbital acquires an occupancy of one and its time reversed companion $\bar{k}_0$ becomes

$$|\phi_{\bar{k}_0}\rangle = a_{\bar{k}_0}^+ \prod_{l \neq \bar{k}_0} (u_l + v_l a_l a_l^\dagger a_l)\bar{u}_l^\dagger \bar{v}_l^\dagger |\bar{-}\rangle$$
empty. Another consequence of blocking, the fact that the odd-A BCS state is no longer invariant under time reversal, makes it more difficult to solve the BCS equations. The Hartree-Fock (HF) and pairing fields also acquire time-odd components which must be included in the HFB energies and minimization procedures.

To avoid dealing with the time-reversal breaking issue, people have made use of the equal filling approximation (EFA). It amounts to replace the density matrix and pairing tensor of a blocked orbital \( k_0 \) by a linear combination with equal weights of the density matrices and pairing tensors of the orbitals \( k_0 \) and \( \bar{k}_0 \). This approximation was widely used even before the whole procedure was justified as a variational problem on the energy of an statistical admixture of the \( k_0 \) and \( \bar{k}_0 \) blocked states \([24]\). Although this procedure gives results which are very close to the real blocking when the time-odd HF and pairing fields are neglected \([25]\), the differences with real blocking can amount to a few hundred KeV and therefore are relevant for the determination of spin and parities of the ground and excited states.

To deal properly with odd-A systems the preferred alternative is the HFB approximation with full blocking. The situation becomes even more involved than the BCS case because now the odd-A wave function is given by

\[
|\phi_{\mu_0}\rangle = \alpha_{\mu_0}^\dagger |\phi\rangle
\]

where \( \alpha_{\mu_0}^\dagger \) is the quasiparticle creation operator of the quasiparticle labeled \( \mu_0 \) and \( |\phi\rangle \) is the wave function of an even number parity reference system. The reference wave function \( |\phi\rangle \) is the vacuum of all the quasiparticle annihilation operators \( \alpha_{\mu} \), i.e. \( \alpha_{\mu} |\phi\rangle = 0 \). On the other hand, \( |\phi_{\mu_0}\rangle \) is the vacuum of the set of quasiparticle operators

\[
\alpha_{1, \ldots, \mu_0 - 1, \mu_0, \mu_0 + 1, \ldots, N}.
\]

The new quasiparticle vacuum can be obtained from the old one \([26, 28]\) by swapping the column \( \mu_0 \) of \( U \) and \( V \). This "swapping" procedure is not very easy to incorporate into a practical implementation of the HFB method for odd-A systems. This is important from a practical standpoint because of odd-A systems typically require many HFB calculations with different starting wave functions in order to insure that the ground state is reached \([29, 30]\). As a consequence, it is very important to have a robust

\(^b\)For spherically orbitals the linear combination runs over the \( 2j + 1 \) sub-levels with weights \( 1/(2j + 1) \)
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and efficient method for solving odd-A systems for global applications such as the construction of theoretical mass table [25, 31, 32].

In the context [33] of generalizing the approximate second order gradient method of [34] it was realized that the “swapping” in the $U$ and $V$ amplitudes can be easily incorporated into the formulas. The argument is as follows: the most important object in the HFB method is the generalized density matrix

$$R = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V^* & U^* \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I} \end{pmatrix} \begin{pmatrix} U^T & V^T \end{pmatrix} = W R W^+ \quad (9)$$

that is given in terms of the unitary Bogoliubov super-matrix

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \quad (10)$$

and the generalized quasi-particle density matrix

$$R_{\nu \mu} = \begin{pmatrix} \langle \phi | \beta^\dagger \beta_{\nu} | \phi \rangle & \langle \phi | \beta_{\mu} \beta^\dagger_{\nu} | \phi \rangle \\ \langle \phi | \beta^\dagger_{\mu} \beta_{\nu} | \phi \rangle & \langle \phi | \beta_{\mu} \beta^\dagger_{\nu} | \phi \rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I}_{\mu_0} \end{pmatrix} \quad (11)$$

When dealing with a blocked HFB state $|\phi_{\mu_0}\rangle$ the generalized quasi-particle density matrix becomes

$$\langle R_{\mu_0}\rangle_{\nu \mu} = \begin{pmatrix} \langle \phi_{\mu_0} | \beta^\dagger_{\mu} \beta_{\nu} | \phi_{\mu_0} \rangle & \langle \phi_{\mu_0} | \beta_{\mu} \beta^\dagger_{\nu} | \phi_{\mu_0} \rangle \\ \langle \phi_{\mu_0} | \beta^\dagger_{\nu} \beta_{\mu} | \phi_{\mu_0} \rangle & \langle \phi_{\mu_0} | \beta_{\mu} \beta^\dagger_{\nu} | \phi_{\mu_0} \rangle \end{pmatrix} = \begin{pmatrix} 0_{\mu_0} & 0 \\ 0 & \mathbb{I}_{\mu_0} \end{pmatrix} \quad (12)$$

where the diagonal matrices $0_{\mu_0}$ and $\mathbb{I}_{\mu_0}$ have been introduced. The first of them, $0_{\mu_0}$ is zero everywhere except in the position $\mu_0$ of the diagonal. The second is the identity matrix except for the element $\mu_0$ of the diagonal that is zero. Using now the trivial matrix identity

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (13)$$

we can write $\langle R_{\mu_0}\rangle$ in terms of $R$

$$\langle R_{\mu_0}\rangle = S_{\mu_0} R S^+_{\mu_0} \quad (14)$$

by means of a ”swapping” matrix $S_{\mu_0}$ that is inspired by the identity of Eq. 13. The effect of $S_{\mu_0}$ acting to the left of the Bogoliubov amplitudes $W$, i.e. $W_{\mu_0} = WS_{\mu_0}$, is to swap the row $\mu_0$ of the $U$ and $V$ amplitudes. The structure of $S_{\mu_0}$ is that of an identity matrix except for the rows and columns of the label $\mu_0$ in both the $U$ and $V$ blocks. The simplifications implied by the introduction of $S_{\mu_0}$ can be seen for instance in the expression of the generalized density

$$R_{\mu_0} = W R_{\mu_0} W^+ = W_{\mu_0} R W^+_{\mu_0}. \quad (15)$$
This tells us that the generalized density can be written in terms of the standard formulas (for instance $\rho = VV^T$), but using the new $U$ and $V$ matrices. More interesting is the variation of the energy at first order when the Bogoliubov amplitudes $W$ are varied according to the most general canonical transformation (see Ref [24] for notation)

$$W(Z) = W(0)e^{iZ}.$$  

where $Z$ is an hermitian bipartite matrix

$$Z = \begin{pmatrix} Z^{11} & Z^{20} \\ -Z^{20*} & -Z^{11*} \end{pmatrix}. \quad (17)$$

The variational parameters of the theory can be enumerated as: the complex matrix off-diagonal elements $Z^{11}_{mn}$ with $m > n$; the diagonal $Z^{11}_{mm}$; and the complex off-diagonal matrix elements $Z^{20}_{mn}$ with $m > n$. The change in energy is given by

$$\delta E = \frac{i}{2} \text{Tr} \left[ [R, H]Z \right] + O(Z^2) \quad (18)$$

with

$$R = W^+(0)HW(0) = \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix}$$

and

$$H = \begin{pmatrix} t + \Gamma & \Delta \\ -\Delta^* - (t + \Gamma)^* \end{pmatrix}.$$  

On the other hand, the change in energy for a blocked HFB state $|\phi_{\mu_0}\rangle$ is given by

$$\delta E_{\mu_0} = \frac{i}{2} \text{Tr} \left[ [R_{\mu_0}, H]Z \right] + O(Z^2) \quad (19)$$

where we have replaced $R$ by $R_{\mu_0}$ and with an $H$ computed from the same density. Using the "swapping" matrix we obtain instead

$$\delta E_{\mu_0} = \frac{i}{2} \text{Tr} \left[ [R, H_{\mu_0}]Z_{\mu_0} \right] + O(Z^2) \quad (20)$$

with $H_{\mu_0} = S_{\mu_0}H S^+_{\mu_0} = W^+_{\mu_0}HW_{\mu_0}$ and $Z_{\mu_0} = S_{\mu_0}ZS^+_{\mu_0}$. For the Bogoliubov amplitudes, the following relation is helpful

$$W(Z)_{\mu_0} = W(0)_{\mu_0}e^{iZ_{\mu_0}}. \quad (21)$$
In practical implementations of the gradient method the exponential in Eq. 21 is computed using the series expansion but corrected to have unitarity. A possibility is
\[ e^{iZ_{\mu_0}} \approx (I + iZ_{\mu_0})(I + Z_{\mu_0}Z_{\mu_0})^{1/2}. \]
where the square root of the positive definite matrix is computed by means of the Cholesky decomposition. Others, based on Padé rational approximations to the exponential have been explored [24].

The previous results are telling us that we can use exactly the same gradient formalism as in the even-even case but using as starting amplitudes $W(0)_{\mu_0}$. Obviously, the idea can be generalized to multiple quasiparticle excitations just by adding as many swapping matrices $S_{\mu_0}$ as quasiparticle excitations considered.

These ideas are being extended to the expansion of the energy up to second order required for a “second order” (Newton like) gradient method and its descendants like the use of the inverse of the sum of quasiparticle energies $E_\mu + E_\nu$ to damp the “high energy” components of the gradient $G_{\mu\nu}$ as discussed in [34]. Although this little trick can not be used for finite temperature systems ($R^2_{\mu_0} = R_{\mu_0}$ is a necessary condition, not satisfied for finite temperature density matrices), work on an efficient implementation of the gradient method using the inverse of two quasiparticle energies as a pre-conditioner and valid for any situation (even-A, odd-A or finite temperature) systems is in progress [33].

4. Conclusions and perspective

Although the standard BCS theory and its use in nuclear physics are both more than fifty years old, there are still technical issues, particularly related to systems with an odd number of particles, that require further developments to simplify the systematic application of BCS/HFB and beyond to nuclear systems all over the nuclide chart. In this contribution we have discussed two of them, one related to the overlaps of HFB wave functions required in theories beyond mean field and using the pfaffian of skew-symmetric matrices. The other focused on the gradient method with blocked HFB wave functions. In the near future, we hope to extend the pfaffian technique to finite temperature systems and make use of it to simplify the application of the generalized Wick theorem. Also, approximate second order gradient methods will be extended to odd-A and finite temperature systems.
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