Chapter 1

Hartree-Fock-Bogoliubov solution of the pairing Hamiltonian in finite nuclei

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We present an overview of the Hartree-Fock-Bogoliubov (HFB) theory of nucleonic superfluidity for finite nuclei. After introducing basic concepts related to pairing correlations, we show how the correlated pairs are incorporated into the HFB wave function. Thereafter, we present derivation and structure of the HFB equations within the superfluid nuclear density functional formalism and discuss several aspects of the theory, including the unitarity of the Bogoliubov transformation in truncated single-particle and quasiparticle spaces, form of the pairing functional, structure of the HFB continuum, regularization and renormalization of pairing fields, and treatment of pairing in systems with odd particle numbers.

1. Introduction

Nucleonic pairing is a ubiquitous phenomenon underlying many aspects of structure and dynamics of atomic nuclei and extended nuclear matter\cite{ref}. The crucial role of nucleonic superfluidity lies in its emergent nature. Indeed, while the correlation energy due to pairing is a small correction to the nuclear binding energy, the superfluid wave function represents an entirely different phase described by new quasiparticle degrees of freedom. The road to this new phase is associated with a phase transition connected with a symmetry breaking, and this underpins the nonperturbative nature
of pairing.

Many facets of nucleonic superfluidity – including those related to phenomenology and theory of pairing – are discussed in this volume. Here, we outline several aspects of nucleonic superfluidity within the framework of the nuclear density functional theory (DFT). The main building blocks of nuclear DFT are the effective mean fields, often represented by local nucleonic densities and currents. When compared to the electronic DFT for the superconducting state, the unique features of the nuclear variant are (i) the presence of two kinds of fermions, protons and neutrons, (ii) the absence of external potential, and (iii) the need for symmetry restoration in a finite self-bound system. In the context of pairing, nuclear superfluid DFT is a natural extension of the traditional BCS theory for electrons and nucleons and a tool of choice for describing complex, open-shell nuclei.

At the heart of nuclear DFT lies the energy density functional (EDF). The requirement that the total energy be minimal under a variation of the densities leads to the Hartree-Fock-Bogoliubov (HFB; or Bogoliubov-de Gennes) equations. The quasiparticle vacuum associated with the HFB solution is a highly correlated state that allows a simple interpretation of various phenomena in the language of pairing mean fields and associated order parameters.

This paper is organized as follows. Section 2 describes the essentials of the general pair-condensate state. The HFB theory is outlined in Sec. 3. The Bogoliubov sea, related to the quasiparticle-quasihole symmetry of the HFB Hamiltonian is discussed in Sec. 4 and Sec. 5 is devoted to the form of the nuclear pairing EDF. The quasiparticle energy spectrum of HFB contains both discrete bound states and continuum unbound states. The properties of the associated quasiparticle continuum are reviewed in Sec. 7. Section 8 describes the extension of the HFB formalism to odd-particle systems and quasiparticle blocking. Finally, conclusions are contained in Sec. 9.

2. Basics of pairing correlations

In quantum mechanics of finite many-fermion systems, pairing correlations are best described in terms of number operators \( \hat{N}_\mu = a_\mu^+ a_\mu \), where \( \mu \) represents any suitable set of single-particle (s.p.) quantum numbers. Thus we may have, e.g., \( \mu \equiv k \sigma \) for plane waves of spin-\( \frac{1}{2} \) particles (electrons); \( \mu \equiv r \sigma \tau \) for spin-\( \frac{1}{2} \) and isospin-\( \frac{1}{2} \) nucleons localized in space at position \( r \); and \( \mu \equiv n, \ell, j, m \) for fermions moving in a spherical potential well. Since
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\[ \hat{N}_\mu = \hat{N}_\mu, \] the number operators are projective; hence, one can – at least in principle – devise an experiment that would project any quantum many-fermion state \(|\Psi\rangle\) into its component with exactly one fermion occupying state \(\mu\). As the rules of quantum mechanics stipulate, any such individual measurement can only give 0 or 1 (these are the eigenvalues of \(\hat{N}_\mu\)), whereas performing such measurements many times, one could experimentally determine the occupation probabilities \(v_\mu^2 = \langle \Psi | \hat{N}_\mu | \Psi \rangle\).

Along such lines, we can devise an experiment that would determine the simultaneous presence of two fermions in different orthogonal s.p. states \(\mu\) and \(\nu\). Since the corresponding number operators \(\hat{N}_\mu\) and \(\hat{N}_\nu\) commute, one can legitimately ask quantum mechanical questions about one-particle occupation probabilities \(v_\mu^2\) and \(v_\nu^2\), as well as about the two-particle occupation. The latter one reflects the simultaneous presence of two fermions in state \(|\Psi\rangle\): \(v_{\mu\nu}^2 = \langle \Psi | \hat{N}_\mu \hat{N}_\nu | \Psi \rangle\). In this way, one can experimentally determine the pairing correlation between states \(\mu\) and \(\nu\) as the excess probability

\[ P_{\mu\nu} = v_{\mu\nu}^2 - v_\mu^2 v_\nu^2, \tag{1} \]

of finding two fermions simultaneously over that of finding them in independent, or sequential, measurements. Such a definition of pairing is independent of its coherence, collectivity, nature of quasiparticles, symmetry breaking, thermodynamic limit, or many other notions that are often associated with the phenomenon of pairing. In terms of occupations, pairing can be viewed as a measurable property of any quantum many-fermion state.

Obviously, no pairing correlations are present in a quantum state that is an eigenstate of \(\hat{N}_\mu\) or \(\hat{N}_\nu\), such as the Slater determinant. The beauty of the BCS ansatz is in providing us with a model \(N\)-fermion state, in which pairing correlations are explicitly incorporated:

\[ |\Phi_N\rangle = \mathcal{N}_N \left( \sum_{\mu > 0} s_\mu z_\mu a_\mu^+ a_\mu^\dagger \right)^{N/2} |0\rangle, \tag{2} \]

where the summation \(\mu > 0\) runs over the representatives of pairs \((\tilde{\mu}, \mu)\) of s.p. states (that is, any one state of the pair is included in the sum, but not both), \(z_{\tilde{\mu}} = z_\mu\) are real positive numbers, \(s_{\tilde{\mu}} = -s_\mu\) are arbitrary complex phase factors, and \(\mathcal{N}_N\) is the overall normalization factor.

It now becomes a matter of technical convenience to employ a particle-
number mixed state,
\[ |\Phi\rangle = \mathcal{N} \sum_{N=0,2,4,\ldots}^{\infty} \frac{|\Phi_N\rangle}{N_N(N/2)!} = \mathcal{N} \exp \left( \sum_{\mu>0} s_\mu z_\mu a_\mu^+ a_\mu^\dagger \right) |0\rangle, \tag{3} \]
in which the pairing correlations (1) are:
\[ P_{\mu\nu} = v_\mu^2 u_\nu^2 \delta_{\mu\nu} \quad \text{for} \quad v_\mu^2 = \frac{z_\mu^2}{1 + z_\mu^2} \quad \text{and} \quad u_\mu^2 = \frac{1}{1 + z_\mu^2}. \tag{4} \]

In terms of the s.p. occupations, the state \( |\Phi\rangle \) assumes the standard BCS form:
\[ |\Phi\rangle = \prod_{\mu>0} \left( u_\mu + s_\mu v_\mu a_\mu^+ a_\mu^\dagger \right) |0\rangle. \tag{5} \]

In this many-fermion state, the s.p. states \( \bar{\mu} \) and \( \mu \) are paired, that is, \( |\Phi\rangle \) can be viewed as a pair-condensate. For \( z_\mu = 1 \), the pairing correlation \( P_{\bar{\mu}\mu} \) equals 1/4; in fact, in this state, it is twice more likely to find a pair of fermions \( (v_\mu^2 = 1/2) \) than to find these two fermions independently \( (v_\bar{\mu}^2 v_\mu^2 = 1/4) \). For particle-number conserving states (2), the occupation numbers can be calculated numerically: qualitatively the results are fairly similar, especially for large numbers of particles.

At this point, we note that the most general pair-condensate state (3) has the form of the Thouless state,
\[ |\Phi\rangle = \mathcal{N} \exp \left( \frac{i}{\hbar} \sum_{\nu\mu} Z^*_{\nu\mu} a_\nu^+ a_\mu^\dagger \right) |0\rangle, \tag{6} \]
in which pairs \( (\bar{\mu}, \mu) \) do not appear explicitly. However, there always exists a unitary transformation \( U_0 \) of the antisymmetric matrix \( Z \) that brings it to the canonical form \( (U_0^+ Z^* U_0^\dagger)_{\nu\mu} = s_\mu z_\mu \delta_{\bar{\mu}\nu} \) (the Bloch-Messiah-Zumino theorem\(^9\)). Therefore, pairs are present in any arbitrary Thouless state (the so-called canonical pairs), and they can be made explicitly visible by a simple basis transformation.

The canonical pairs exist independently of any symmetry of the Thouless state. In the particular case of a time-reversal-symmetric state, \( \hat{T} |\Phi\rangle = |\Phi\rangle \), they can be associated with the time-reversed s.p. states, \( \bar{\mu} \equiv \mu \). The ground-states of even-even nuclei can be described in this manner. However, the appearance of pairing phase does not hinge on this particular symmetry – states in rotating nuclei (in which time-reversal symmetry is manifestly broken) can also be paired. In this latter case the canonical states are less useful, because they cannot be directly associated with the eigenstates of the HFB Hamiltonian.
3. Hartree-Fock-Bogoliubov theory

The simplest route to the HFB theory is to employ the variational principle to a two-body Hamiltonian using Thouless states as trial wave functions. The variation of the average energy with respect to the antisymmetric matrix $Z$ results in the HFB equation in the matrix representation,

$$\mathcal{H}U = UE,$$

or explicitly,

$$(T + \Gamma \Delta - \Delta^* - T^* - \Gamma^*) (UV^*) = (E_0 - E) (UV^*),$$

where $T_{\mu\nu}$ is the matrix of the one-body kinetic energy, $\Gamma_{\mu\nu} = \sum_{\mu'} V_{\mu'\mu\nu'} \rho_{\nu\nu'}$ and $\Delta_{\mu\nu} = \frac{1}{2} \sum_{\nu\nu'} V_{\mu\nu',\nu\nu'} \kappa_{\nu\nu'}$ are the so-called particle-hole and particle-particle mean fields, respectively, obtained by averaging two-body matrix elements $V_{\mu\nu',\nu\nu'}$ with respect to the density matrix $\rho_{\nu\nu'} = \langle \Phi | a^+_\nu a_{\nu'} | \Phi \rangle$ and pairing tensor $\kappa_{\nu\nu'} = \langle \Phi | a^+_\nu a_{\nu'} | \Phi \rangle$, and $E$ is the diagonal matrix of quasiparticle energies.

The matrices $\mathcal{H}$ and $U$ are referred to as the HFB Hamiltonian and Bogoliubov transformation, respectively, and columns of $U$ (eigenstates of $\mathcal{H}$) are vectors of quasiparticle states. The HFB equation (7) possesses the quasiparticle-quasihole symmetry. Namely, for each quasiparticle state $\chi_\alpha$ (the $\alpha$-th column of $U$) and energy $E_\alpha$ there exists a quasihole state $\phi_\alpha$ of opposite energy $-E_\alpha$,

$$\chi_\alpha = (U_{\mu \alpha} V_{\mu \alpha}), \quad \phi_\alpha = (V^*_{\mu \alpha} U^*_{\mu \alpha}).$$

That is, the spectrum of $\mathcal{H}$ is composed of pairs of states with opposite energies. In most cases, the lowest total energy is obtained by using the eigenstates with $E_\alpha > 0$ as quasiparticles $\chi_\alpha$ and those with $E_\alpha < 0$ as quasiholes $\phi_\alpha$, that is, by occupying the negative-energy eigenstates. States $\chi_\alpha$ and $\phi_\alpha$ can usually be related through a self-consistent discrete symmetry, such as time reversal, signature, or simplex.

The HFB equation (7) is also valid in a more general case, when the total energy is not equal to the average of any many-body Hamiltonian. Within the DFT, it stems from the minimization of the binding energy given by an EDF $\mathcal{E}(\rho, \kappa, \kappa^*)$, subject to the condition of the generalized density matrix being projective, that is, $\mathcal{R}^2 = \mathcal{R}$ for

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} = \begin{pmatrix} V^* VT & V^* U^T \\ U^* VT & U^* UT \end{pmatrix} = \begin{pmatrix} V^* \\ U^* \end{pmatrix} \begin{pmatrix} VT & UT \end{pmatrix} = \sum_\alpha \phi_\alpha \phi_\alpha^*.$$
In this case, the mean fields are obtained as functional derivatives of EDF:
\[ \Gamma_{\mu\nu} = \frac{\partial E}{\partial \rho_{\nu\mu}} \] and \[ \Delta_{\mu\mu'} = \frac{\partial E}{\partial \kappa_{\mu\mu'\ast}}. \] As is the case in DFT, densities (here the density matrix and pairing tensor) become the fundamental degrees of freedom, whereas the state \(|\Phi\rangle\) acquires the meaning of an auxiliary entity (the Kohn-Sham state). Indeed, for any arbitrary generalized density matrix \( R \), one can always find the corresponding state \(|\Phi\rangle\). For that, one determines the Bogoliubov transformation \( U \) as the matrix of its eigenvectors, \( RU = U \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \); the Thouless state \(|\Phi\rangle \) corresponds to \( Z = VU^{-1} \). Consequently, the paired state \(|\Phi\rangle\) of DFT is not interpreted as a wave function of the system – it only serves as a model for determining one-body densities. Nonetheless, these densities are interpreted as those associated with the (unknown) exact eigenstate of the system.

Unrestricted variations of the EDF are not meaningful. Indeed, since Thouless states are mixtures of components with different particle numbers, absolute minima will usually correspond to average particle numbers that are unrelated to those one would like to describe. In particular, for self-bound systems governed by attractive two-body forces (nuclei), by adding more and more particles one could infinitely decrease the total energy of the system. Therefore, only constrained variations make sense, that is, one has to minimize not the total energy \( E(\rho, \kappa, \kappa_{\ast}) \), but the so-called Routhian, \( E'(\rho, \kappa, \kappa_{\ast}) = E(\rho, \kappa, \kappa_{\ast}) + C(\rho) \), where \( C \) is a suitably chosen penalty functional, ensuring that the minimum appears at prescribed average values of one-body operators. In particular, the average total number of particles can be constrained by \( C(\rho) = -\lambda \langle \Phi | \hat{N} | \Phi \rangle = -\lambda \text{Tr}(\rho) \) (linear constraint) or \( C(\rho) = C_N[\text{Tr}(\rho) - N_0]^2 \) (quadratic constraint), where \( \lambda \) becomes the Fermi energy corresponding to \( N_0 \) fermions.

For different systems and for different applications, various constraints \( C(\rho) \) can be implemented; for example, in nuclei one can simultaneously constrain numbers of protons and neutrons, as well as multipole moments of matter or charge distributions. When the total energy is a concave function of relevant one-body average values, quadratic constraints are mandatory. The minimization of \( E'(\rho, \kappa, \kappa_{\ast}) \) requires solving the HFB equation for the quasiparticle Routhian \( \mathcal{H}' \), which, for the simplest case of the constraint on the total particle number, reads \( \mathcal{H}' = \mathcal{H} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \).

Finally, let us mention that in the coordinate space-spin(-isospin) representation, the HFB equation acquires particularly interesting form, which in condensed matter and atomic literature is called Bogoliubov-de
Gennes equation[4] In the coordinate representation, quasiparticle vectors become two-component wave functions, which – in finite systems – acquire specific asymptotic properties[15][21] determining the asymptotic behavior of local densities. The quasiparticle energy spectrum of HFB contains discrete bound states, resonances, and non-resonant continuum states. As illustrated in Fig. 1 the bound HFB solutions exist only in the energy region \(|E_i| \leq -\lambda\). The quasiparticle continuum with \(|E_i| > -\lambda\) consists of non-resonant continuum and quasiparticle resonances, see Sec. 6.

![Fig. 1. Quasiparticle spectrum of the HFB Hamiltonian. The bound states exist in the energy region \(|E_i| \leq -\lambda\), where \(\lambda\) is the chemical potential (always negative for a particle-bound system).](image)

4. Beneath the bottom of the Bogoliubov sea

Because of the quasiparticle-quasihole symmetry (Sec. 3), the spectrum of the HFB Hamiltonian contains as many negative as positive eigenvalues. Therefore, the HFB equation (7) constitutes an eigenvalue problem for the
operator unbounded from below, and the HFB spectrum extends from minus to plus infinity, see Fig. 1. Moreover, one-body densities (density matrix and pairing tensor) are given by infinite sums over all negative-energy (quasihole) states, cf. Eq. (9). In analogy to the Fermi sea of occupied states, which appears in the Hartree-Fock (HF) theory, we call the set of quasihole states the Bogoliubov sea. Note again that the Fermi sea extends over a finite range of energies – from the bottom of the HF potential up to the Fermi energy – whereas the Bogoliubov sea is infinitely deep, in a nice analogy with the sea of one-electron states of the relativistic Dirac equation.

In practice, since infinite sums over the Bogoliubov sea cannot be carried out, the number of pairing-active states must be truncated. Two different ways of achieving this goal are most often implemented, namely, solution of the HFB equations in a finite s.p. space (e.g., the so-called two-basis method) and truncation of the summation in the quasiparticle space. The second method correspond to creating an artificial finite bottom of the Bogoliubov sea. In this section we discuss the consequences of neglecting the quasihole states that are below the bottom of that sea.

The main problem concerns the calculation of the pairing tensor, which is the sum of products of upper and lower components of quasihole states, cf. Eq. (9). When this sum is performed over the infinite complete set of quasiparticle states, the resulting pairing tensor is antisymmetric, while for truncated sums it may acquire a symmetric part. Usually the symmetric component is small; hence, can be neglected. However, its very existence means that the many-fermion state which would have had such a pairing tensor simply does not exist. The smallness of the symmetric part can be deceiving, because the symmetric pairing tensor corresponds to a many-boson system. Consequently, appearance of the symmetric component implies the violation of the Pauli principle. This is a potentially dangerous situation – within a variational theory one should avoid the boson sector whose ground state is way below the fermionic ground state.

A solution to this problem, discussed below, consists in marrying the two truncation methods mentioned above. That is, we shall first use the quasiparticle truncation method to define the appropriate s.p. cutoff, and then the HFB equations are solved in this truncated space, leading to a perfectly antisymmetric pairing tensor.

Let us consider the case of truncated summations over the Bogoliubov sea and assume that we have kept only $K$ quasihole states. In order to maintain the quasiparticle-quasihole symmetry, we apply the same truncation
to quasiparticle and quasihole states, that is, we also keep $K$ quasiparticle
partner states. This is convenient, and always possible, because the quasipar-
ticle (unoccupied) states do not impact HFB densities. Then, matrix $\mathbf{U}$
becomes rectangular – it has less columns ($2K$) than rows. Since all kept
quasiparticle and quasihole states are orthonormal, we still have $\mathbf{U}^T\mathbf{U} = 1$.
However, since now the quasiparticle space is not complete, $\mathbf{U}$ is not any-
more unitary, and the product $\mathbf{U}\mathbf{U}^+ = \mathcal{P}$ is not equal to unity. All what
remains is the hermitian and projective property of $\mathcal{P}$:

$$\mathcal{P}^+ = \mathcal{P}, \quad \mathcal{P}^2 = \mathcal{P}. \tag{10}$$

Since $\text{Tr}\mathcal{P} = 2K$, $\mathcal{P}$ has exactly $2K$ eigenvalues equal to 1.

In its explicit form, matrix $\mathcal{P}$ reads:

$$\mathcal{P} = \begin{pmatrix} P & Q \\ Q^* & P^* \end{pmatrix} = \begin{pmatrix} UU^+ + V^*V^T, UV^+ + V^*U^T \\ VV^+ + U^*V^T, VV^+ + U^*U^T \end{pmatrix}. \tag{11}$$

In terms of $P$ and $Q$, Eqs. (11) can be written as:

$$P^+ = P, \quad Q^T = Q \quad \text{and} \quad P^2 + QQ^+ = P, \quad PQ + QP^* = Q, \tag{12}$$

where $\text{Tr}P = K$.

Properties of matrices $P$ and $Q$ can be most easily discussed in the
particle basis that diagonalizes $P$. Suppose that column $f$ is an eigenvector
of $P$ with eigenvalue $p$, that is, $Pf = pf$. From Eqs. (12) it follows that $p$
must be between 0 and 1. Moreover, if $Qf^*$ is not equal to zero, then $Qf^*$
is an eigenvector of $P$ with eigenvalue $1 - p$, that is, $P(Qf^*) = (1 - p)Qf^*$.
Conversely, if $Qf^*$ is equal to zero, than $p = 0$ or $p = 1$.

Altogether, the spectrum of $P$ can be divided into three regions: (i)
$i$ states with $p_i = 1$, where all matrix elements of $Q$ vanish, $Q_{\nu\nu'} = 0$, (ii)
$2k$ states with $0 < p_\nu < 1$, where eigenvectors are arranged in pairs $p_\nu = 1 - p_\nu$
such that the only non-vanishing matrix elements of $Q$ are

$$Q_{\nu\nu} = Q_{\nu'\nu} = q_\nu = \sqrt{p_\nu(1 - p_\nu)}, \tag{13}$$

and (iii) states with $p_\nu = 0$, where again all matrix elements of $Q$ vanish. In
practical calculations of solving the HFB equation in infinite-dimensional
quasiparticle spaces (like the coordinate representation), the first region
almost never appears ($i = 0$), and then $k = K$. However, for truncated
quasiparticle spaces, the third region always exists and contains the null
space of $P$.

We now see that when $K$ quasiparticles are included in the quasiparticle
space and $i = 0$, in the particle space there appears a basis of $2K$ s.p. states,
which we call natural basis. Each state in the first half of the natural basis has its partner in the second half. By ordering the eigenvalues of $P$ and neglecting the zero eigenvalues for $\nu > 2K$, we can write matrices $P$ and $Q$ in a general form:

$$
P = \begin{pmatrix}
    p_1 & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
    0 & p_2 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & \ldots & p_K & 0 & 0 & \ldots & 0 \\
    0 & 0 & \ldots & 0 & 1-p_K & 0 & \ldots & 0 \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & \ldots & 0 & 0 & 1-p_2 & \ldots & 0 \\
    0 & 0 & \ldots & 0 & 0 & 0 & \ldots & 1-p_1 \\
\end{pmatrix}, \\
Q = \begin{pmatrix}
    0 & 0 & \ldots & 0 & 0 & 0 & \ldots & q_1 \\
    0 & 0 & \ldots & 0 & q_2 & 0 & \ldots & 0 \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & \ldots & 0 & q_K & 0 & \ldots & 0 \\
    0 & 0 & \ldots & 0 & 0 & 1-q_K & \ldots & 0 \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & q_2 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
    q_1 & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
\end{pmatrix}.
$$

(14)

If there appear $i > 0$ states with $p_\nu = 1$, the number of paired states decreases to $2k = 2K - 2i$ and the size of the natural basis decreases to $i + 2k = 2K - i$.

The HFB equations can now be solved in the finite natural basis, whereupon the pairing tensor becomes exactly antisymmetric and the dangerous violations of the Pauli principle are removed exactly\cite{23}. The advantage of this method is in the fact that the truncated s.p. space is not arbitrarily cut but it is adjusted to the truncated quasiparticle space.

5. Pairing functional

The form of the most general pairing EDF that is quadratic in local isoscalar and isovector densities has been discussed in Refs.\cite{25,26}. Because of the lack of nuclear observables that can constrain coupling constants of this general pairing functional, current realizations are much simpler. A commonly used effective pairing interaction is the zero-range pairing force with the density-dependent form factor:\cite{27–31}

$$
\rho_{\sigma}(r) = V_0 \left\{ 1 + x_0 \hat{P}_\sigma - \left[ \frac{\rho_0(r)}{\rho_c} \right]^{\alpha} (1 + x_3 \hat{P}_d) \right\},
$$

(15)

where $\hat{P}_\sigma$ is the usual spin-exchange operator and $\rho_0=0.16 \text{fm}^{-3}$. When only the isovector pairing is studied, the exchange parameters $x_0$ and $x_3$ are usually set to 0. However, in the general case of coexisting isoscalar and isovector pairing correlations, nonzero values of $x_0$ and $x_3$ have to be used. Pairing interactions corresponding to $\eta=0$, 0.5, and 1, are usually referred to as volume, mixed, and surface pairing, respectively.\cite{32–34} The
volume pairing interaction acts primarily inside the nuclear volume while the surface pairing generates pairing fields peaked around or outside the nuclear surface.

Another form of density dependence has been suggested in Ref. 35 and successfully applied 36 to explain odd-even effects in charge radii. As discussed in Refs. 31,37 different assumptions about the density dependence may result in differences of pairing fields in very neutron rich nuclei. However, the results of the global survey 38 suggest that – albeit there is a slight favoring of the surface interaction – one cannot reliably extract the density dependence of the effective pairing interaction (15) from the currently available experimental odd-even mass differences, limited to nuclei with a modest neutron excesses (see also Refs. 34,39,40).

A timely question, related to the density dependence, is whether there is an effective isospin dependence of the pairing interaction. The global survey 38 of odd-even staggering of binding energy indicates that the effective pairing strength $V_0$ for protons is larger than for neutrons, and the recent large-scale optimizations of the nuclear EDF are consistent with this finding 41,42. This can be attributed to the isospin-dependent contribution to pairing from the Coulomb interaction 43–45 or to induced pairing due to the coupling to collective excitations 46,47.

To account for those effects, an extended density dependence has been proposed 48–50 that involves the local isovector density $\rho_1(r)$.

Little is known about the isoscalar pairing functional. The local isovector pairing potential 25,26 $\vec{U}(r)$ is proportional to the isovector pair density $\vec{\rho}$ whereas the isoscalar pairing potential $\vec{\Sigma}_0(r)$ is a vector proportional to the isoscalar-vector pairing spin density $\vec{s}_0$. Then, the isoscalar pairing field,

$$\vec{h}_0(r) = \vec{\Sigma}_0 \cdot \vec{\sigma} \propto \vec{s}_0 \cdot \vec{\sigma}$$

is the projection of the quasiparticle’s spin on the proton-neutron pairing field. Physically, $\vec{\rho}$ represents the density of $S=0$, neutron-neutron, proton-proton, and proton-neutron pairs, whereas the vector field $\vec{s}_0$ describes the spin distribution of $S=1$ pn pairs (that is, it contains all magnetic components of $S=1$ pn pairing field).

Symmetries of the isoscalar pairing mean-fields have been studied in detail in Ref. 26. As an example, lines of the solenoidal field $\vec{s}_0$ – present in the generalized pairing theory that mixes proton and neutron orbits – are schematically shown in Fig. 2. It is interesting to note that for the geometry of Fig. 2 the third component $\vec{s}_{0z}$, associated with the $M=0$ isoscalar...
pairing field vanishes. That is, the solenoidal pairing field is created by the two components with $M = \pm 1$. One can thus conclude that the assumption of axial symmetry, or signature, does not preclude the existence of isoscalar pairing.

![Diagram](image)

Fig. 2. (a) Schematic illustration of the isoscalar vector pairing field $\mathbf{s}_0$ in the case of conserved axial and mirror symmetries. The field is solenoidal, with vanishing third component. (b) Under rotation around the third (symmetry) axis, the field at the point $r_A$ is transformed to the position $r_B$. Likewise, under $R_x$, the field is transformed to $r_C$. While neither of these operations leave the individual vector $s_0(r_A)$ invariant, the field as whole does not change.

6. Pairing and the HFB continuum

The structure of HFB continuum indicated schematically in Fig. 1 has been a subject of many works. Within the real-energy HFB framework, the proper theoretical treatment of the HFB continuum is fairly sophisticated since the scattering boundary conditions must be met. One way of tackling this problem is the coordinate-space Green’s function technique. If the outgoing boundary conditions are imposed, the unbound HFB eigenstates have complex energies; their imaginary parts are related to the particle width. The complex-energy spherical HFB problem has been formulated and implemented within the Gamow HFB (GHFB) approach of Ref.

In addition to the methods that directly employ proper asymptotic boundary conditions for unbound HFB eigenstates, the quasiparticle con-
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The continuum of HFB can be approximately treated by means of a discretization method. The commonly used approach is to impose the box boundary conditions in the coordinate-space calculations, in which wave functions are spanned by a basis of orthonormal functions defined on a lattice in coordinate space and enforced to be zero at box boundaries. In this way, referred to as the $L^2$ discretization, quasiparticle continuum of HFB is represented by a finite number of box states. It has been demonstrated by explicit calculations for weakly bound nuclei that such a box discretization is accurate when compared to the exact results. Alternatively, diagonalizing the HFB matrix in the Pöschl-Teller-Ginocchio basis or Woods-Saxon basis turned out to be an efficient way to account for the continuum effects. Finally, quasiparticle continuum can be effectively discretized by solving the HFB problem by means of expansion in a harmonic oscillator (HO) or transformed HO (THO) basis. As far as the description of nonlocalized HFB states is concerned, the coordinate-space method is superior over the HO expansion method, as the HO basis states are always localized. Consequently, the discretized representation of the quasiparticle continuum is different in coordinate-space and HO basis-expansion approaches.

Among the quasiparticle resonances, the deep-hole states play a distinct role. In the absence of pairing, a deep-hole excitation with energy $E_i > 0$ corresponds to an occupied HF state with energy $\varepsilon_i = -E_i + \lambda$. If pairing is present, it generates a coupling of this state with unbound particle states with $\varepsilon_i \approx E_i + \lambda$ that gives rise to a quasiparticle resonance with a finite width. Quasiparticle resonance widths can be directly calculated with a high precision using coordinate-space Green’s function technique and GHFB. For approaches based on the $L^2$ discretization, several approximate methods have been developed to deal with HFB resonances. The modified stabilization method based on box solutions has been used to obtain precisely the resonance energy and widths. Based on the box solutions, the HFB resonances are expected to be localized solutions with energies weakly affected by changes of the box size. The stabilization method allows to obtain the resonance parameters from the box-size dependence of quasiparticle eigenvalues.

Besides the stabilization method, a straightforward smoothing and fitting method that utilizes the density of box states has been successfully used. In this technique, resonance parameters are obtained by fitting the smoothed occupation numbers obtained from the dense spectrum discretized HFB solutions. Figure displays occupation probabilities $v_i^2$ for
Fig. 3. Occupation numbers of the discretized neutron quasiparticle continuum states calculated for $^{70}\text{Zn}$ in Ref.\textsuperscript{57} The corresponding Breit-Wigner envelopes are indicated by dashed lines. The $-\lambda_n$ threshold is marked by a dotted line.

the discretized neutron quasiparticle states in $^{70}\text{Zn}$ as a function of quasiparticle energy $E_i$. To extract resonance parameters from the discrete distribution of $\nu_i$, one can first smooth it using a Lorentzian shape function and then perform a fit using a Breit-Wigner function.\textsuperscript{57}

Various ways of computing widths of high-energy deep-hole states have been compared in Ref.\textsuperscript{57} By comparing with the exact GHFB results, it has been concluded that the stabilization method works fairly well for all HFB resonances, except for the very narrow ones. The smoothing-fitting method is also very effective and can easily be extended to the deformed case. The perturbative Fermi golden rule\textsuperscript{20} has been found to be unreliable for calculating widths of neutron resonances. (For more discussion on limitations of the perturbative treatment, see Ref.\textsuperscript{20}).

Pairing correlations can profoundly modify properties of the system in
drip line nuclei due to the presence of the vast continuum space available for pair scattering. One example is the appearance of the pairing-antihalo effect, in which pairing correlations in the weakly-bound even-particle system change the asymptotic behavior of particle density thus reducing its radial extension. While neutron radii of even-even nuclei are expected to locally increase when approaching the two-neutron drip line, the size of the resulting halo is fairly modest, especially when compared with spatial extensions of neighboring odd-neutron systems.

Pairing correlations impact the limits of the nuclear existence: the odd-even staggering of the nuclear binding energy does result in the shift between one-neutron and two-neutron drip lines. The pairing coupling to the positive-energy states is an additional factor influencing the nuclear binding. In particular, because of strong coupling to the neutron continuum, the neutron chemical potential may be significantly lowered thus extending the range of bound nuclei, and this effect is expected to depend on the character of pairing interaction. For more discussion on the impact of continuum on quasiparticle occupations, emergence of bound canonical HFB states from the continuum, and contributions of nonresonant continuum to the localized ground state in dripline nuclei, see Refs.

7. Regularization of the local pairing interaction

As discussed in Sec. 5 in many HFB applications, pairing interaction is often assumed to be in the form of the zero-range, density-dependent force. Calculations using the contact interaction are numerically simpler, but the pairing gap diverges when the dimension of the pairing-active space increases for a fixed strength of the interaction. In roots of this problem is the ultraviolet divergence of abnormal density for zero-range pairing interaction:

$$\tilde{\rho}(r - x/2, r + x/2) \sim - \frac{\hbar}{4\pi\hbar^2|x|} \left|M^*(r)\right|_{x \to 0}. \quad (17)$$

Consequently, in practical calculations, one has to apply a cutoff procedure to truncate the pairing-active space of s.p. states, and the pairing strength has to be readjusted accordingly. Thus the energy cutoff and the pairing strength together define the pairing interaction, and this definition can be understood as a phenomenological introduction of finite range. Such a sharp cut-off regularization is performed in the
spirit of the effective field theory, whereupon contact interactions are used to describe low-energy phenomena while the coupling constants are readjusted for any given energy cutoff to account for high energy effects. It has been shown that by an appropriate renormalization the pairing strength for each value of the cutoff energy, one practically eliminates the dependence of various observables on the cutoff parameter. Figure 4 illustrates the procedure for the total energy in the tin isotopes. While for a fixed pairing strength total energies depend significantly on the cut-off energy (top), for a fixed pairing gap the changes obtained with renormalized interactions (bottom) are very small indeed.

![Figure 4](image-url)

Fig. 4. Total energies in the tin isotopes calculated within the HFB+SkP$^\delta$ model. Top panel shows the results for the fixed interaction strength $V_0$ and for several cut-off energies $\Delta E_{\text{max}}$ added to the usual $\ell j$-dependent cut-off energy $E_{\text{max}}$. Bottom panel shows similar results when the values of $V_0$ are renormalized to keep the average neutron pairing gap in $^{120}\text{Sn}$ the same for each $\Delta E_{\text{max}}$.

The cutoff energy dependence of the pairing strength can also be handled by means of a regularization scheme by defining the regularized local abnormal density:

$$\tilde{\rho}_r(r) = \lim_{x \to 0} [\tilde{\rho}(r-x/2, r + x/2) - f(r, x)], \quad (18)$$

where $f$ is a regularization counterterm, which removes the divergence at $x = 0$. For cutoff energies high enough, one can express $f$ through the s.p.
Green’s function at the Fermi level, \( G(r + x/2, r - x/2) \), which also exhibits a \( 1/x \) divergence. In practical calculations, one can use the Thomas-Fermi (TF) approximation for the local s.p. Green’s function; this approach has been used with success for a description of spherical and deformed nuclei.\(^{37,54,86,87}\) As demonstrated in Ref.\(^{54}\) the differences between pairing renormalization and regularization procedures are rather small.

A combination of the renormalization and regularization methods described above is the hybrid technique\(^ {57}\) based on the TF approximation to the non-resonant HFB continuum.\(^{88,89}\) This approach is of great practical interest as it makes it possible to carry out calculations in wide pairing windows and very large coordinate spaces. In the hybrid method, the high-energy continuum above the cutoff energy \( E_c \) is divided into the non-resonant part and deep-hole states. While deep-hole states have to be treated separately, the non-resonant continuum contribution to HFB densities and fields can be integrated out by means of the TF approximation. The choice of the cutoff \( E_c \) is determined by positions of deep-hole levels\(^ {57}\); this information can be obtained by solving the HF problem.

### 8. Pairing in odd-mass nuclei

The zero-quasiparticle HFB state (6), representing the lowest configuration for a system with even number of fermions, corresponds to a filled sea of Bogoliubov quasiholes with negative quasiparticle energies, see Fig. 1. In a one-quasiparticle state representing a state in an odd nucleus, a positive-energy quasiparticle state \( \alpha \) is occupied and its conjugated quasihole partner is empty. The corresponding wave function can be written as

\[
|\Phi^{(\alpha)}_{\text{odd}}\rangle = \mathcal{N}_{\alpha}^+ \exp \left( \frac{1}{2} \sum_{\nu\mu} Z_{\nu\mu} a_{\nu}^+ a_{\mu}^- \right) |0\rangle,
\]

where \( \alpha^+_\alpha \) is the quasiparticle creation operator,

\[
\alpha^+_\alpha = \sum_{\nu} (U_{\nu\alpha} a_{\nu}^+ + V_{\nu\alpha} a_{\nu}),
\]

which depends on the quasiparticle state \( \chi_{\alpha} \). Density matrix and pairing tensor of state (19) can be obtained by exchanging in \( \mathcal{U} \) columns corresponding to the quasiparticle and quasihole states, \( \chi_{\alpha} \) and \( \phi_{\alpha} \). The corresponding density matrix reads explicitly,

\[
\rho^{(\alpha)}_{\mu\nu} = (V^* V^T)_{\mu\nu} + U_{\mu\alpha} U_{\nu\alpha}^* - V_{\mu\alpha}^* V_{\nu\alpha},
\]
and similar holds for the pairing tensor. After the column replacement, matrix \( U^{(\alpha)}_{\mu\alpha} \) of one-quasiparticle state becomes singular and has null space of dimensions one. Hence, the occupation number of one of the s.p. states equals to 1. This fact is at the origin of the name “blocked states” attributed to one-quasiparticle states (19). These states contain fully occupied s.p. states that do not contribute to pairing field.

The blocking can also be implemented, for some configurations, by introducing two chemical potentials for different superfluid components (two-Fermi level approach, 2FLA95,96 As demonstrated in Ref.93 such procedure is equivalent to applying a one-body, time-odd field that changes the particle-number parity of the underlying quasiparticle vacuum. For polarized Fermi systems, in which no additional degeneracy of quasiparticle levels is present beyond the Kramers degeneracy, the 2FLA is equivalent to one-dimensional, non-collective rotational cranking.

When describing properties of odd-mass nuclei, one selects the lowest quasiparticle excitations \( E_\alpha \) and carries out the self-consistent procedure based on these blocked candidates (19). Naturally, one must adopt a prescription to be able to determine, at each iteration, the index \( \alpha \) of the quasiparticle state to be blocked97 Such a unique identification can be done by means of, e.g., the overlap method of Ref.98 After the HFB iterations are converged for each blocked candidate, the state corresponding to the lowest energy is taken as the ground state of an odd-mass nucleus, and the remaining ones are approximations of the excited states. A similar procedure can be applied to many-quasiparticle states, e.g., two-quasiparticle states in even-even and odd-odd nuclei, three-quasiparticle excited states in odd-mass nuclei, and so on.

The state (19) represents an odd-Fermi system that carries nonzero angular momentum; hence, it breaks the time reversal symmetry. If the time reversal symmetry is enforced, additional approximations have to be applied based on the Kramers degeneracy. One of them is the equal filling approximation (EFA), in which the degenerate time-reversed states \( \chi_\alpha \) and \( \chi_{\bar{\alpha}} \) are assumed to enter the density matrix and pairing tensor with the same weights94,99 For instance, the blocked density matrix of EFA reads:

\[
\rho^{\text{(EFA)}}_{\mu\nu}(\alpha) = (V^* V^T)_{\mu\nu} + \frac{1}{2} \left( U_{\mu\alpha} U_{\nu\alpha}^* - V_{\mu\alpha} V_{\nu\alpha}^* + U_{\mu\bar{\alpha}} U_{\nu\bar{\alpha}}^* - V_{\mu\bar{\alpha}} V_{\nu\bar{\alpha}}^* \right). \tag{22}
\]

It has been shown100 that the EFA and the exact blocking are both strictly equivalent when the time-odd fields of the energy density functional are put to zero. Thus, EFA is adequate in many practical applications that do not require high accuracy.
Although for the functionals restricted to time-even fields, the time-reversed quasiparticle states $\alpha$ and $\bar{\alpha}$ are exactly degenerate, this does not hold in the general case. Here, the blocking prescription may depend on which linear combination of those states is used to calculate the blocked density matrix. This point can be illuminated by introducing the notion of an $\textit{alispin}$, which describes the arbitrary unitary mixing of $\chi_\alpha$ and $\chi_\bar{\alpha}$: $\chi'_\alpha = a\chi_\alpha + b\chi_\bar{\alpha}$ ($|a|^2 + |b|^2 = 1$). As usual, the group of such unitary mixings in a $2 \times 2$ space can be understood as rotations of abstract spinors, which we here call alirotations of alispinors. If the time-reversal symmetry is conserved, the blocked density matrix becomes independent of the mixing coefficients $(a, b)$, that is, it is an aliscalar. In the general case where time-reversal symmetry is not dynamically conserved, however, the blocked density matrix is not aliscalar. Here, the blocked density matrix may depend on the choice of the self-consistent symmetries and the energy of the system may change with alirotation.

The key point in this discussion is the realization that blocking must depend on the orientation of the alignment vector with respect to the principal axes of the mass distribution. To determine the lowest energy for each quasiparticle excitation, self-consistent calculations should be carried out by varying the orientation of the alignment vector with respect to the principal axes of the system. While in many practical applications one chooses a fixed direction of alignment dictated by practical considerations, it is important to emphasize that it is only by allowing the alignment vector to point out in an arbitrary direction that the result of blocked calculations would not depend on the choice of the basis used to describe the odd nucleus. Illuminating examples presented in Ref. demonstrate that the choice of the alignment orientation does impact predicted time-odd polarization energies.

Examples of self-consistent HFB calculations of one-quasiparticle states can be found in Refs. (full blocking) and Refs. (EPA).

9. Summary and conclusions

The superfluid DFT based on self-consistent HFB has already become the standard tool to describe pairing correlations in atomic nuclei. Such framework has been implemented in numerous approaches aiming at a consistent description of particle-hole and particle-particle channels, and it is gradually replacing a much simpler original BCS theory. This is so, because in finite systems like nuclei, spatial dependence of particle and pairing fields
has to be properly described, especially in the nuclear periphery of weakly bound isotopes. In this respect, the BCS theory and its different flavors are manifestly deficient. In this study, we aimed at presenting some basics of the local superfluid DFT along with several aspects of it related to advanced current applications. There are, of course, numerous aspects of the HFB theory that we could not cover in this limited overview. First, there have been many applications of the HFB theory using finite-range interactions, which imply nonlocal pairing fields. While they are significantly more difficult to treat, they do not lead to ultraviolet divergencies. Based on the current description of the limited set of nuclear observables related to pairing, it is difficult to judge whether the finite range is essential. In fact, one can understand finite-range interactions in terms of regularized local functionals. Second, we did not discuss various issues related to the restoration of particle-number symmetry. Effects of particle-number nonconservation are probably little significant in heavy nuclei, but they may become crucial for some observables and in specific systems, like, for example, nuclei with only few particles in valence shells. Third, we could not cover subjects related to the treatment of pairing in high-spin states where the broken time-reversal symmetry precludes the use of the BCS theory. Fourth, pairing correlations impact nuclear dynamics in a profound way. Recently, there have been many exciting developments related to the treatment of small- and large-amplitude collective motion in weakly-bound superfluid nuclei. Finally, we did not discuss details of the HFB theory applied to the isoscalar pairing. This channel becomes essential in nuclei with almost equal numbers of protons and neutrons, and numerous applications of the HFB theory to this case exist in the literature, see Refs. Many of these topics are discussed in other contributions contained in this Volume.

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