The BCS-to-BEC crossover, as well as the nature of Cooper pairs, in superconducting and Fermi superfluid media is studied from the exact ground state wavefunction of the reduced BCS Hamiltonian. As the strength of the interaction increases, the ground state continuously evolves from a mixed-system of quasifree fermions and pair resonances (BCS), to pair resonances and quasibound molecules (pseudogap), and finally to a system of quasibound molecules (BEC). A single unified scenario arises where the Cooper-pair wavefunction has a unique functional form. Several exact analytic expressions such as the binding energy and condensate fraction are derived. We compare our results with recent experiments in ultracold atomic Fermi gases.

The nature of Cooper pairs in the BCS-BEC crossover has regained attention due to the observation of a large fraction of preformed fermion pairs on the BCS side of the Feshbach resonance in ultracold atomic Fermi gases \[1\]. While several theoretical explanations were proposed \[2\], the interpretations are still controversial. The root of the controversy is understanding what represents a Cooper pair in a correlated Fermi system, a concept not clearly defined in the literature. This paper discusses this concept at the very foundational level and proposes a qualitatively different scenario of the BCS-BEC crossover, based on the exact solution to the BCS Hamiltonian \[3\]. Only in the extreme BEC limit does this new scenario and Leggett’s naive ansatz \[4\] become identical.

While the superconducting and Fermi superfluid thermodynamic states represent a mixed-system of quasifree and pair-correlated fermions, the molecular BEC which arises in the dilute and strong coupling limit has all fermions bound into pairs forming a unique macroscopic quantum state. It is by now well accepted in which sense these states represent a Bose-Einstein (BE) condensation. What defines a BE condensation in an interacting \(N\)-particle system is spontaneous gauge symmetry breaking, or phase coherence, of its quantum state (a concept that strictly applies in the thermodynamic limit (TL)). Yang \[5\] provided a detailed mathematical characterization of this phenomenon which manifests itself as off-diagonal long-range order (ODLRO) or, equivalently, by the existence of an eigenvalue of order \(N\) in a reduced density matrix \(\hat{\rho}_n\), where \(n\) is the number of particles forming the smallest unit that condenses.

The above definition of a BEC does not imply the naive view of a many-body state of quantum objects with identical internal wavefunctions. Indeed, we will argue that a currently-carrying mean-field ground state (GS) of a uniform superconducting or Fermi superfluid \(N\)-particle system is of the form

\[
\Psi(x_1, \cdots, x_N) = A \left[ \phi_1(x_1, x_2) \cdots \phi_{N/2}(x_{N-1}, x_N) \right],
\]

with \(x_j = (r_j, \sigma_j)\), antisymmetrizer \(A\), and the pair state

\[
\phi_\alpha(x_i, x_j) = e^{i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)} \varphi_\alpha(r_{ij}) \chi(\sigma_i, \sigma_j),
\]

where \(\chi\) is a spin function of a certain symmetry, \(\mathbf{q}\) is the pair center-of-mass momentum, and \(\varphi_\alpha(r)\) the internal wavefunction which may represent either a quasimolecular resonant state or a scattering state (i.e., a mixed state), depending upon the strength of the interaction between particles.

For pedagogical reasons we will recall the one-Cooper-pair problem and then address the question of what happens when we add more pairs (\(q = 0\) in the GS). The Cooper-pair solution can be recovered from the wavefunction \(|\Psi\rangle\) by assuming that \(N - 2\) fermions \(c^\dagger_k \sigma\) are free, filling the lowest momentum states \(k\) (of energy \(\varepsilon_k\)) up to the Fermi momentum \(k_F\), while only an additional fermion pair (with momenta \(k > k_F\)) feels an attractive s-wave interaction in the spin singlet channel

\[
|\Psi\rangle_c = \sum_{k > k_F} \frac{1}{2\varepsilon_k - \Delta} |k\uparrow c^\dagger_{-k\downarrow} F\rangle.
\]

The role of the Fermi sea, \(|F\rangle = \prod_{k < k_F} c^\dagger_k c^\dagger_{-k}\rangle |0\rangle\), is to Pauli-block states below the Fermi energy \(\varepsilon_{k_F}\). Assuming that the attractive pairing interaction \(G < 0\) is constant around the Fermi energy, the eigenvalue \(E\) is always negative implying that the Cooper pair is bound regardless of the strength of the attractive interaction. The Fermi sea is then unstable against the formation of bound pairs of electrons.

What happens when the pairing interaction also affects electrons in the Fermi sea? The answer to this question is the BCS theory whose canonical form considers a state of the form \(|\Psi\rangle\) with all identical internal wavefunctions

\[
\hat{P}_M|\text{BCS}\rangle = (\Lambda^\dagger)^M|0\rangle, \quad \Lambda^\dagger = \sum_{\mathbf{k}, \mathbf{k}' \neq \mathbf{0}} \frac{v_{\mathbf{k}}}{|v_{\mathbf{k}}|} c_{\mathbf{k}}^\dagger c_{\mathbf{k}'}^\dagger c_{-\mathbf{k}'} c_{-\mathbf{k}},
\]

where \(\hat{P}_M\) is the projector onto the state with \(M\) pairs, and \(v_{\mathbf{k}}, u_{\mathbf{k}}\) are the BCS amplitudes \(\left|\frac{v_{\mathbf{k}}^2}{u_{\mathbf{k}}^2}\right| = \frac{1}{2} \left[ 1 \mp \frac{\Delta - \mu}{\sqrt{\left(\varepsilon_{\mathbf{k}} - \mu\right)^2 + \Delta^2}} \right]\) with \(\Delta\) the gap and \(\mu\) the chemical potential. Since the structure of the BCS pair is averaged over the whole system, it does not characterize a Cooper pair in the superconducting medium except in the extreme strong-coupling and dilute limits where all pairs are bounded and non-overlapping. Sometimes, the structure of the Cooper pair is associated with the pair-correlation function \(\text{BCS}\left|c_{\mathbf{k}}^\dagger c_{\mathbf{k}'}^\dagger\right| = u_{\mathbf{k}} v_{\mathbf{k}}\) describing the pair correlation among fermions of the same pair as well as the exchange between fermions of different pairs.
proposed by Richardson 40 years ago \cite{ Richardson, BCS}. \( H \) involves all terms with time-reversed pairs \((k, -k)\) from a contact interaction. It is consistent with an effective single-channel description of the BCS-BEC crossover theory \cite{ BCS} in terms of a zero-range potential. Realistic finite-range interactions produce qualitatively similar results along the crossover \cite{ Cooper}.

For simplicity we will consider \( N = N_1 + N_{-1} \) spin-1/2 (i.e., 2-flavor) fermions in a three-dimensional box of volume \( V \) with periodic boundary conditions, interacting through an attractive constant \((s\text{-wave-singlet-pairing})\) potential. (Other pairing symmetries can also be accommodated.) Exact \( N = 2M + \nu \) particle eigenstates of \( H \) can be written as

\[
|\Psi\rangle = \prod_{\ell=1}^{M} S^+_{\ell}|\nu\rangle, \quad S^+_{\ell} = \sum_{k>0} \frac{1}{2\varepsilon_k - E_\ell} c_{\ell k}^\dagger c_{k\ell}^\dagger, \quad (6)
\]

where \( |\nu\rangle \equiv |\nu_1, \nu_2, \cdots, \nu_L\rangle \) is a state of \( \nu \) unpaired fermions \((\nu = \sum_k \nu_k, \text{with } \nu_k = 1, 0)\) defined by \( c_{k\ell}|\nu\rangle = 0\), and \( \nu_k|\nu\rangle = \nu_k|\nu\rangle \). \( L \) is the total number of single particle states. The GS \( |\Psi_0\rangle \) is in the \( \nu = 0 \) \((N_1 = N_{-1})\) sector.

Each eigenstate \( |\Psi\rangle \) is completely defined by a set of \( M \) (in general, complex) spectral parameters (pair energies) \( E_\ell \) which are a solution of the Richardson’s equations

\[
1 + \frac{G}{V} \sum_{k>0} \frac{1-\nu_k}{2\varepsilon_k - E_\ell} + \frac{G}{V} \sum_{m(\neq \ell)} \frac{1}{E_\ell - E_m} = 0, \quad (7)
\]

and the eigenvalues of \( H \) are \( \mathcal{E} = \sum_{k} \varepsilon_k c_{k\ell}^\dagger c_{k\ell} + \sum_{\ell=1}^{M} E_\ell \) \cite{ Cooper, BCS}. A crucial observation is that if a complex \( E_\ell \) satisfies \( 4\pi \varepsilon_e \), its complex-conjugate \( \overline{E_\ell} \) is also a solution. Thus, \(|\Psi\rangle \) restores time-reversal invariance. The ansatz \cite{ Cooper} is a natural generalization of the Cooper-pair problem without an inert Fermi sea, and with all pairs subjected to the pairing interaction. The pair structure in \cite{ Cooper} is similar to the Cooper pair in \cite{ Cooper}, and the many-body state has the form \cite{ Cooper} with all pairs different.

Since we are concerned with uniform bulk Fermi systems, we are interested in the TL (i.e., \( N, V \rightarrow \infty \) with \( \rho = N/V = k_B^3/\pi^2 = \text{constant} \)). This limit was studied by Gaudin \cite{ Gaudin} when the energy spectrum \( \Omega \in [\omega, \omega] \) is bounded, and \( \nu = 0 \). Eqs. \cite{ Cooper} reduce to the well-known gap equation

\[
\frac{1}{2} \int_{\Omega} d\varepsilon \frac{g(\varepsilon)}{\sqrt{(\varepsilon - \mu)^2 + \Delta^2}} + \frac{1}{G} = 0, \quad (8)
\]

where \( g(\varepsilon) \) represents the density of states. In our case \( \Omega \in [0, \infty) \) is unbounded with \( g(\varepsilon) = m^{3/2}/(\sqrt{2}\pi^2\hbar^3) \) for \( \varepsilon_k = \hbar^2 k^2/2m \). Due to the absence of an upper cutoff, Eq. \cite{ Cooper} is singular and the TL becomes a subtle mathematical procedure whose solution will be presented here \cite{ Cooper}. 

| \( \eta \) | \( \mu \) | \( \Delta \) | \( \mathcal{E}_B \) | \( \lambda \) |
|---|---|---|---|---|
| \( -\infty \) | \( 1 + \left(\frac{\eta}{\eta} - \frac{\eta}{\Delta} \right) \Delta^2 \) | \( \frac{\Delta^2}{\eta} \) | \( \frac{3\pi}{8} \frac{\exp\left(\eta\right)}{\eta^2} \) | \( \frac{2}{\pi} \frac{\exp\left(\eta\right)}{\eta^2} \)|
| 0 | \( \frac{\sqrt{1-x^2}}{E(\sqrt{1-x^2})} \) | \( \frac{\sqrt{2\eta}}{\eta} \) | \( \frac{\sqrt{2\eta}}{\eta} \) | \( \frac{3\pi}{8} \frac{\exp\left(\eta\right)}{\eta^2} \) |
| \( +\infty \) | \( -\eta^2 \) | \( \frac{20\pi}{\eta^2} \) | 2\( \eta^2 \) | 1 |

**TABLE I:** Analytic expressions for selected values of \( \eta = 1/k_F a_s \); \( x \) is the root of \( P_a \), i.e. \( P_a(0) = 0 \), and \( E(\eta) \) is the complete elliptic integral of the second kind. Note that \( 5\pi^2 \mathcal{E}_0(\eta = 0)/k_F^2 = \mu(\eta = 0) \approx 0.500606 \).

There are two ways to regularize the problem: One can either introduce an energy cutoff in the integrals or one can cancel the singularities with physical quantities whose bare counterpart diverges in the same way \cite{ Cooper}. For this problem, Eq. \cite{ Cooper}, the physical quantity is the scattering length \( a_s \) given by

\[
\frac{m}{4\pi\hbar^2 a_s} = \frac{1}{G} + \frac{1}{2} \int_{0}^{\infty} d\varepsilon \frac{g(\varepsilon)}{\varepsilon}. \quad (9)
\]

The non-singular gap equation (after integration \cite{ Cooper}) is

\[
\frac{1}{k_F a_s} = \eta = \sqrt{\mu^2 + \Delta^2} P_\Delta \left( -\frac{\mu}{\sqrt{\mu^2 + \Delta^2}} \right), \quad (10)
\]

where energies are now in units of \( \varepsilon_F = \hbar^2 k_F^2/2m \) and lengths in units of \( \xi_F = 1/k_F \). \( P_\beta(x) \) is the Legendre function of the first kind of degree \( \beta \). The equations for the conservation of the number of pairs \( M \)

\[
-\frac{4}{3\pi} = \eta \mu + (\mu^2 + \Delta^2)^{3/4} P_\Delta \left( -\frac{\mu}{\sqrt{\mu^2 + \Delta^2}} \right), \quad (11)
\]

and GS energy density, for arbitrary strength \( \eta \),

\[
\mathcal{E}_0 = \frac{-1}{V} \langle \Psi_0 | \mathcal{H} | \Psi_0 \rangle = -\frac{k_F^3}{20\pi} \left[ \frac{\eta^2}{2} - \frac{4}{\pi} \frac{\mu}{\mu - 4} \right], \quad (12)
\]

do not need regularization, these are exact results. Indeed, for a given \( \eta \), the chemical potential \( \mu \) and gap \( \Delta \) need to be determined self-consistently from Eqs. \cite{ Cooper} and \cite{ Cooper} (Fig. 1). Then, the GS energy can be computed as a function of density using Eq. \cite{ Cooper}. It shows no phase segregation. The exact binding (or condensation) energy per electron pair \( \mathcal{E}_B \) is (see Table I)

\[
\mathcal{E}_B = \frac{3\pi}{10} \left[ \frac{\eta^2}{2} - \frac{4}{\pi} \frac{\mu}{\mu - 1} \right]. \quad (13)
\]

The complete solution of Eqs. \cite{ Cooper} in the TL \cite{ Cooper} amounts to determining (for a given \( \eta \)) the set of pair energies \( E_\ell \) which, for the GS, form a single open, continuous, and reflection-symmetric arc \( \Gamma \) with extreme points \( \bar{E}_F = 2(\mu \pm i\Delta) \). Here, we simply present the results without derivation. The equation for \( \Gamma \) is
fraction $f = 0.35$, and $\eta = 0$ (dashed line) with $f = 0.87$. The pseudogap region $P$, indicated in light grey, extends from $\eta = 0.37$ to $\eta = 0.55$ where $\mu = 0$. Within this region the real part of the pair energies changes from positive to negative, and $P$ describes a mixture of Cooper resonances and quasibound molecules. The BEC (white) region, $\eta > 0.55$, is characterized by all pair energies having negative real parts, i.e., all pairs are quasibound molecules. As $\eta$ increases further, $\Gamma$ tends to an almost vertical line with $\text{Re}(E) \sim 2\mu$, and $-2\Delta \leq \text{Im}(E) \leq 2\Delta$.

If the literature is not clear about the size $\xi$ of a Cooper pair, it is partly because it is not clear what a Cooper pair is. Pippard, in his nonlocal electrodynamics of the superconducting state, introduced the characteristic length $\xi_0$ by using an uncertainty-principle argument involving only electrons within a shell of width $2\Delta$ around the Fermi energy. The resulting quantity, named Pippard’s coherence length, $\xi_0 = 2/(\pi \Delta)$, is usually associated to $\xi$. On the other hand, an acceptable definition could be $\xi = \sqrt{\langle \phi|\phi \rangle} / \langle \phi | \phi \rangle = 1$.

From Eq. (14), the Cooper-pair wavefunction is

$$\varphi_E(r) = \frac{1}{\sqrt{V}} \sum_k \varphi_k^E e^{ikr} = A \frac{e^{-r\sqrt{E/2}}}{r},$$

with $A^2 = \text{Im}(\sqrt{E/2})/2\pi \xi_0^2$, $\varphi_k^E = C/(2\epsilon_k - E)$, and $C$ being a normalization constant. Thus, $\xi_E = 1/\text{Im}(\sqrt{E})$. In the weak-coupling BCS limit ($\Delta \ll \mu \approx 1$), when $E = E_F$, we get $\xi_E = \pi \xi_0 / \sqrt{2}$. On the other hand, in the same limit, if one uses $\varphi_k^P = C \rho_{\text{p}} k_{\text{p}} \xi_0$, one gets $\xi_P = \xi_E / 2$, and if one uses $\varphi_k^{\text{BCS}} = C \rho_{\text{BCS}} \epsilon_k / \mu_k$, one gets $\xi_{\text{BCS}} = \sqrt{2} \xi_E / 2$.

![FIG. 2: Different definitions of Cooper-pair sizes $\xi$, and condensate fraction $\lambda$ and $f$ as a function of the interaction strength $\eta$. The horizontal solid line represents the interparticle distance $r_\Lambda = \sqrt{9\pi/4.}](image)

Analytic expressions (using dimensional regularization) for $\xi_P$ and $\xi_{\text{BCS}}$ can also be obtained for arbitrary coupling strength. Figure 2 displays the different sizes, all labelled by $\xi$, as a function of $\eta$. Clearly, in $\xi_P$ there is no unique pair size $\xi_P$ but a distribution of sizes; Fig. 2 shows in solid line the smallest size in $\Gamma$ corresponding to $E_F$. On the other hand, there is a unique pair size for $\varphi_P$ and $\varphi_{\text{BCS}}$; the dashed
and dotted lines correspond to the $\xi_p$ and $\xi_{\text{BCS}}$ sizes respectively. Notice the relation between sizes and the interparticle distance $r_s = \sqrt{3}/4\pi$ which is indicated as a full horizontal line. While $\xi_E$ and $\xi_p$ increase for negative $\eta$ values, and eventually diverge when $\eta \to -\infty$, $\xi_{\text{BCS}}$ tends to a constant value, related to the interparticle distance, showing its essentially uncorrelated nature. The fact that $\xi_p < \xi_E/2$ in the overlapping BCS region is a clear demonstration that $\xi_p$ measures the mean distance between time-reversed pairs irrespective of the Cooper pair they belong to. For non-overlapping pairs (BEC region) both sizes converge to the same values.

![Graph showing Cooper-pair sizes and distribution](image)

**FIG. 3:** Cooper-pair sizes $\xi_E$ along the arcs $\Gamma$ for the values of $\eta$ depicted in Fig. 1.

Following Yang [5], ODLRO in $\hat{\rho}_2(r_1 \uparrow r_2 \downarrow | r_3 \uparrow r_4 \downarrow) \rightarrow \phi^* (r_1 \uparrow, r_2 \downarrow) \phi (r_3 \uparrow, r_4 \downarrow)$ may be used to define

$$
\lambda = \frac{2}{N} \int dr_1 dr_2 |\phi (r_1 \uparrow, r_2 \downarrow)|^2 = \frac{3\pi}{16 \text{Im}(\mu + i\Delta)} \quad (16)
$$

as a measurement of the condensate fraction. Figure 2 shows $\lambda$ and the fraction $f$ of (Cooper) pairs in the arc, that is, the fraction of complex spectral parameters. Although $\lambda$ can qualitatively describe the fraction of correlated pairs, the fraction $f$ gives the value 1 at the BCS-pseudogap boundary ($\eta = 0.37$) while $\lambda = 1$ for $\eta \to \infty$. We note that at resonance ($\eta = 0$), $f = 87\%$ of the fermions form Cooper pairs ($\lambda \approx 0.7$). These results provide a qualitative explanation of the experiments in [1] without resorting to a projection method [8]. Close to resonance on the BCS side, a fraction $f \approx 80\%$ of the atoms form Cooper pairs with sizes comparable to $r_s$. Those atom pairs are efficiently transformed into quasimolecules during a rapid magnetic field ramping across the resonance giving rise to the molecular condensate fractions observed experimentally.

One may argue that selecting the smallest pair from each arc to compare (in Fig 2) Cooper-pair sizes along the crossover might not be representative of the Cooper-pair distribution within each arc. In Fig. 4 we show the internal variations of the pair sizes within the arcs. Although in the BCS region there is a distribution of sizes from the smallest pair with $E = E_F$ in the extremes of the arc to an almost infinite size pairs when they are close to the real axis, already at resonance ($\eta = 0$) most of the pairs have the same structure. This latter feature becomes more pronounced in the BEC region.

The various definitions of Cooper-pair wavefunctions are depicted in Fig. 4 which compares $\varphi_{\text{BCS}}(r)$, $\varphi_p(r)$, and $\varphi_E(r)$ for interaction strengths which correspond to the BCS, Feshbach resonance, and BEC regions of Fig. 1. Notice that while $\varphi_{\text{BCS}}$, $\varphi_p$ are highly oscillatory in the weak-coupling region, this is not the case with $\varphi_E$ which always has an exponential form. Clearly, a single and unified picture emerges for the crossover when using a many-body state such as $\Psi$: $\varphi_E$ evolves smoothly through the crossover as it should. It is important to mention that the three wavefunctions are exactly the same in the strong coupling limit $\eta \to +\infty$. In this limit the naive ansatz of Leggett [4] and the GS coincide, becoming a simple Pfaffian state.

![Graph showing Cooper-pair wavefunctions](image)

**FIG. 4:** Cooper-pair wavefunctions for different $\eta$. The upper and middle (Feshbach resonance) panels correspond to the BCS region, while the bottom one is in the BEC region. Except for the Cooper $\varphi_E$ case, the other two wavefunctions always vanish at $r = 0$. It is only in the limit $\eta \to +\infty$ that the three states exactly coincide.

In summary, we studied the BCS-BEC crossover problem, as well as the nature of Cooper pairs in a correlated Fermi system, from the exact GS $|\Psi_0\rangle$ of the reduced BCS Hamiltonian. We have analytically determined its exact TL for the quadratic single-particle dispersion, and calculated several quantities of physical interest, such as the binding (or condensation) energy and the condensate fraction. The validity of the present description is not restricted to integrable pairing Hamiltonians, but rather the ansatz $|\Psi_0\rangle$, which is a natural extension of the Cooper problem, could be used as a variational state for more realistic interactions. The Cooper-pair wavefunc-
tion $\varphi_E$ has a fixed functional $s$-wave form that accommodates pair-correlated fermions close to the Fermi energy in the weak coupling limit as well as quasibound molecules in the BEC limit. It is free from the characteristic oscillations displayed by $\varphi_{BCS}$ and $\varphi_P$ related to exchange among pairs. The BCS region in the crossover diagram represents a mixture of Cooper pairs and quasifree fermions. It may be argued that the single-channel model is insufficient to describe the system close to resonance where the degrees of freedom associated to the molecular closed channel should be explicitly incorporated. A derivation analogous to the one presented here can be pursued by using a recently proposed atom-molecule integrable model \cite{12} which captures the essential features of the two-channel model \cite{13}. The structure of the Cooper pair in this new model is the same as in \cite{6}.

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