Cooper pairs as resonances

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Abstract

Using the Bethe-Salpeter (BS) equation, Cooper pairing can be generalized to include contributions from holes as well as particles from the ground state of either an ideal Fermi gas (IFG) or of a BCS many-fermion state. The BCS model inter-fermion interaction is employed throughout. In contrast to the better-known original Cooper pair problem for either two particles or two holes, the generalized Cooper equation in the IFG case has no real-energy solutions. Rather, it possesses two complex-conjugate solutions with purely imaginary energies. This implies that the IFG ground state is unstable when an attractive interaction is switched on. However, solving the BS equation for the BCS ground state reveals two types of real solutions: one describing moving (i.e., having nonzero total, or center-of-mass, momenta) Cooper pairs as resonances (or bound composite particles with a finite lifetime), and another exhibiting superconducting collective excitations analogous to Anderson-Bogoliubov-Higgs RPA modes. A Bose-Einstein-condensation-based picture of superconductivity is addressed.

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1. Introduction

The original Cooper pair (CP) equation \[ \frac{\delta}{\delta a_{k\sigma}} \] is a two-electron Schrödinger equation in momentum representation with a given two-body interaction (having some attraction) but includes ad hoc restrictions on the magnitudes of both electron wavevectors \( k_1, k_2 \), namely \( k_1 > k_F, k_2 > k_F \), where \( k_F \) is the electron Fermi wavenumber for an ideal nonrelativistic many-electron system. One then seeks the energy eigenvalues of a CP bound state and its corresponding wavefunction.

Since there is no rigorous derivation of the original CP equation, several authors reformulated the complete CP problem without neglecting holes, using the mathematically exact BS equation approach applied to the system, in search of two-particle bound states in the presence of other system electrons. Such a treatment allows generalizing several approaches in superconductivity theory, including the BCS, the BCS-Bose crossover, and the Bose-Einstein condensation pictures. But if the BS equation is based merely on the IFG ground state one obtains purely imaginary solutions, suggesting that the ground state is unstable in the presence of attractive interactions of some kind. This is an instability of the IFG ground state with respect to the creation of two-particle (2p-) or two-hole (2h-) resonant states, a situation analogous to the classical problem of hydrodynamic instability.

2. BS equation based on BCS ground state

Consider, however, the generalized two-component, two-electron BS equation based not on the IFG ground state but rather on the BCS ground state. We introduce the Bogoliubov-Valatin \( u, v \) transformation of electron Fermi operators \( a_{k\sigma} \) to new Fermi operators \( a_{k\sigma} \), namely

\[
\begin{align*}
a_{k\sigma} &= u_k a_{k\sigma} + 2\sigma v_k \alpha_{-k,-\sigma}^+, \\
\end{align*}
\]

where \( \sigma = \pm \frac{1}{2} \) is the spin projection for an electron state. The coefficients \( u_k, v_k \) are real and depend on \( k \). The many-electron system hamiltonian is \( H = H_0 + H_{int} \) where

\[
H_0 = \sum_{k\sigma} (\epsilon_k - E_F) a_{k\sigma}^+ a_{k\sigma},
\]
\[ H_{int} = \frac{1}{2L^3} \sum'_{k_1,k_2,k_1',k_2',\sigma_1,\sigma_2} \nu(|k_1 - k_1'|) \times \]
\[ \times a_{k_1',\sigma_1}^+ a_{k_2,\sigma_2}^+ a_{k_2,\sigma_2} a_{k_1,\sigma_1}, \] (2)

where \( \epsilon_k = \hbar^2 k^2 / 2m \) is the kinetic energy of an electron of mass \( m \); \( E_F = \hbar^2 k_F^2 / 2m \) is the Fermi energy; \( L \) is the system size; \( \nu(q) \) the Fourier transform of the two-electron interaction potential; and the last sum is restricted by momentum conservation \( k_1 + k_2 = k_1' + k_2' \). This leads to the well-known BCS Hamiltonian

\[ H_{BCS} = U_0 + \sum_{k,\sigma} E(k) a_{k,\sigma}^+ a_{k,\sigma}, \] (3)

with \( U_0 \) a generalized BCS ground-state energy

\[ U_0 = 2 \sum_k (\epsilon_k - E_F) v_k^2 + \]
\[ + L^{-3} \sum_{k,k'} \nu(|k - k'|) v_k u_k v_k u_{k'} + \]
\[ + 2L^{-3} \sum_{k,k'} \nu(0) v_k^2 v_{k'}^2 - L^{-3} \sum_{k,k'} \nu(|k - k'|) v_k^2 v_{k'}^2, \]

where

\[ u_k^2 = \frac{1}{2} \left[ 1 + \frac{A(k)}{E(k)} \right], \quad v_k^2 = \frac{1}{2} \left[ 1 - \frac{A(k)}{E(k)} \right], \]
\[ 2 u_k v_k = - \frac{B(k)}{E(k)}, \quad E(k) = \sqrt{A^2(k) + B^2(k)}. \] (4)

Here \( B(k) \) plays the role of the original BCS energy gap \( \Delta(k) \), and

\[ A(k) \equiv \epsilon_k - E_F + \]
\[ + 2L^{-3} \nu(0) \sum_{k'} v_{k'}^2 - L^{-3} \sum_{k'} \nu(|k - k'|) v_{k'}^2, \]
\[ B(k) \equiv L^{-3} \sum_{k'} \nu(|k - k'|) u_{k'} v_{k'}. \] (5)

For the new interaction Hamiltonian we obtain

\[ H_{int}' = H - H_{BCS} = \]
\[ = \frac{1}{2L^3} \sum'_{k_1',k_2',k_1,k_2,\sigma_1,\sigma_2} \nu(|k_1 - k_1'|) \times \]
\[ \times L(k_1,k_1') L(k_2,k_2') \times \]
\[ \times a_{k_1',\sigma_1}^+ a_{k_2,\sigma_2}^+ a_{k_2,\sigma_2} a_{k_1,\sigma_1}, \]
\[ + \frac{1}{4L^3} \sum'_{k_1',k_2',k_1,k_2,\sigma_1,\sigma_2} \nu(|k_1 - k_1'|) \times \]
\[ \times M(k_1,k_1') M(k_2,k_2') \times \]
\[ \times 2 \nu(k_1') a_{k_1',\sigma_1}^+ a_{k_1,\sigma_1}^+ a_{k_2,\sigma_2}^+ a_{k_2,\sigma_2}, \]
\[ + \frac{1}{4L^3} \sum'_{k_1',k_2',k_1,k_2,\sigma_1,\sigma_2} \nu(|k_1 - k_1'|) \times \]
\[ \times M(k_1,k_1') M(k_2,k_2') \times \]
\[ \times 2 \nu(k_1') a_{k_1',\sigma_1}^+ a_{k_1,\sigma_1}^+ a_{k_2,\sigma_2} a_{k_2,\sigma_2}, \]
\[ + \frac{1}{4L^3} \sum'_{k_1',k_2',k_1,k_2,\sigma_1,\sigma_2} \nu(|k_1 - k_1'|) \times \]
\[ \times M(k_1,k_1') M(k_2,k_2') \times \]
\[ \times 2 \nu(k_1') a_{k_1',\sigma_1}^+ a_{k_1,\sigma_1} a_{k_2,\sigma_2}^+ a_{k_2,\sigma_2}, \]
\[ + \frac{1}{4L^3} \sum'_{k_1',k_2',k_1,k_2,\sigma_1,\sigma_2} \nu(|k_1 - k_1'|) \times \]
\[ \times M(k_1,k_1') M(k_2,k_2') \times \]
\[ \times 2 \nu(k_1') a_{k_1',\sigma_1} a_{k_1,\sigma_1}^+ a_{k_2,\sigma_2}^+ a_{k_2,\sigma_2}. \]

where \( L(k,k') \equiv u_k v_k' - v_k u_k' \) and \( M(k,k') \equiv u_k v_k' + u_k' v_k \).

To obtain the BS equation based on the BCS ground state consider the Feynman diagrams of perturbation theory based on this ground state, where (B) is the new unperturbed hamiltonian \( H_0' \). We now have the usual arrowed electron lines labeled by \( \mathbf{k} \), \( E \), \( \sigma \) to which we associate the BCS unperturbed Green's function

\[ G_0(k,E,\sigma) = \frac{\hbar}{i - E + E(k) - i \epsilon}, \] (6)

where \( E(k) \) is given by (4). There exist four-line-end double vertices of six different kinds (see Fig. 1) where the interference interaction is denoted by
dashed lines. To a double vertex type (a) of Fig. 1, with two outgoing line ends with indices \((k_1', E_1', \sigma_1)\) and \((k_2', E_2', \sigma_2)\) along with two incoming line ends with indices \((k_1, E_1, \sigma_1)\) and \((k_2, E_2, \sigma_2)\), we attach the factor
\[
-L^{-3} \nu(|k_1 - k_1'|) L(k_1, k_1') L(k_2, k_2').
\]
To a double vertex of type (b), with two outgoing line ends \((k_1', E_1', \sigma_1)\) and \((k_2', E_2', \sigma_2)\) along with two outgoing line ends \((-k_1, -E_1, -\sigma_1)\) and \((-k_2, -E_2, -\sigma_2)\), as well as to a double vertex of type (c) with two incoming line ends with indices \((-k_1', -E_1', -\sigma_1)\) and \((-k_2', -E_2', -\sigma_2)\) along with two incoming line ends with indices \((k_1, E_1, \sigma_1)\) and \((k_2, E_2, \sigma_2)\), we attach the factor
\[
-L^{-3} \nu(|k_1 - k_1'|) 4\sigma_1\sigma_2 M(k_1, k_1') M(k_2, k_2').
\]

![Image](image.png)

**FIG. 1.** Six different types of vertices with corresponding topological automorphism factors \(g\).

### 3. Coupled BS equations

Because of different kinds of vertices in Fig. 1 we now have a system of two coupled BS equations. Figure 2 shows their diagrammatic representation in the ladder approximation of the two-electron BS equation for the BCS ground state. Depicted are both the two-electron \(\psi_+(kE; K\varepsilon_K)\) and two-hole \(\psi_-(kE; K\varepsilon_K)\) bound-state functions. Here \(K \equiv k_1 + k_2\) is the total (or center-of-mass) wave-vector and \(\varepsilon_K\) is the total energy of the two electrons referred to \(2E_F\).

Using the diagrammatic rules just described, the two-component BS equations for the bound state is
\[
\psi_+(kE') = -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE' L^{-3} \sum_{k'} \nu(|k - k'|) \times L(K/2 + k, K/2 + k') L(K/2 - k, K/2 - k') \times (i/\hbar)^2 \mathcal{G}_0 (K/2 + k, \varepsilon_K/2 + E) \times \mathcal{G}_0 (K/2 - k, \varepsilon_K/2 - E) \psi_+(k' E') -
\]
\[
\times M(K/2 + k, K/2 + k') M(K/2 - k, K/2 - k') \times (i/\hbar)^2 \mathcal{G}_0 (K/2 + k, \varepsilon_K/2 + E) \times \mathcal{G}_0 (K/2 - k, \varepsilon_K/2 - E) \psi_-(k' E');
\]
\[
(7)
\]
\[
\psi_-(kE) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE' L^{-3} \sum_{k'} \nu(|k - k'|) \times L(K/2 + k, K/2 + k') L(K/2 - k, K/2 - k') \times (i/\hbar)^2 \mathcal{G}_0 (-K/2 - k, -\varepsilon_K/2 - E) \times \mathcal{G}_0 (-K/2 + k, -\varepsilon_K/2 + E) \psi_-(k' E') -
\]
\[
\times M(K/2 + k, K/2 + k') M(K/2 - k, K/2 - k') \times (i/\hbar)^2 \mathcal{G}_0 (-K/2 - k, -\varepsilon_K/2 - E) \times \mathcal{G}_0 (-K/2 + k, \varepsilon_K/2 + E) \psi_+(k' E').
\]
\[
(8)
\]
It can be shown that these equations coincide exactly with those used in the description of collective excitations in the BCS-Bogoliubov microscopic theory of superconductivity.

![Image](image2.png)

**FIG. 2.** Diagrammatic representation of the two-component coupled BS equations.
4. CP solutions of BS equations

We now employ the BCS model interaction

$$\nu(|k - k'|) = -(k_F^2/k^2)^2 V \eta(k)\eta(k'),$$  \hspace{1cm} (9)

where $V \geq 0$, and $\eta(k) = 1$ when $k_F - k_D < k < k_F + k_D$ and $= 0$ otherwise. Here $k_D \equiv m \omega_D/hk_F$ with $\omega_D$ the Debye frequency, if $h \omega_D < \hbar F_F$.

The detailed solution for the system of the two-component coupled BS equations of Fig. 2 is too cumbersome to present here, but it can be shown that they yield two types of independent solutions. The first solution of (7) and (8) with (9) is just

$$\omega|K\rightarrow(K_t/2)^2$$

This gives

$$t = \cos \theta. \quad \text{The integral over the polar angle } \theta \text{ is restricted to from } 0 \text{ to } \pi/2 \text{ since the integrand in } (10) \text{ vanishes for } t < 0. \text{ We first integrate over } k \text{ from } k_{\text{min}} \text{ to } k_{\text{max}} \text{ which are solutions of } |K_t/2 + k| = k_F, \text{ and } |K_t/2 - k| = k_F, \text{ or}

$$k_{\text{min}} = -K_t/2 + \sqrt{K_t^2/4 - K^2/4 + k_F^2},
$$k_{\text{max}} = K_t/2 + \sqrt{K_t^2/4 - K^2/4 + k_F^2}.$$

The restrictions $k_F - k_D \leq k \leq k_F + k_D$ are not illustrated in Fig. 3 as they are unimportant for us. As $K \rightarrow 0$ we then have

$$k_{\text{min}} \approx -K_t/2 + O(K^2),
$$k_{\text{max}} \approx K_t/2 + O(K^2),
$$E(|K/2 + k|) + E(|K/2 - k|) \approx 2 \Delta + O(K^2)

where we redefined the integration variable $k = k_F + xK$, with $x$ the new variable.

![FIG. 3. Integration region in (11)](image)

Consequently in seeking a solution of Eq. (11), for example of the form

$$\mathcal{E}_K = 2 \Delta + c hK + O(K^2),$$

where $c$ is a constant, we obtain for small $\Delta$ and $K$

$$\frac{V k_F^2}{4 \pi^2 \hbar} \int_0^1 dt \int_{k_F - Kt/2}^{k_F + Kt/2} \frac{dk}{cK} \approx 1.$$

Thus $c = V k_F^2/8 \pi^2 \hbar$. Finally one gets

$$\mathcal{E}_K = 2 \Delta + \frac{\lambda}{4} v_F hK + O(K^2),$$  \hspace{1cm} (12)
together with its symmetric solution

\[ \varepsilon_K = -2\Delta - \frac{\lambda}{4} v_F hK + O(K^2), \tag{13} \]

where \( \lambda \equiv N(0)V \) and \( N(0) \equiv m k_F / 2\pi^2 h^2 \). These two solutions describe moving 2p-CPs and 2h-CPs, respectively. A linear-in-\( K \) behavior of the moving pair binding energy was obtained for the original Cooper-pair problem \([1]\) but it was independent of the interaction coupling strength as it excluded 2\( h \)-CP contributions. More significantly, the binding energy there was negative as it refers to an infinite-lifetime composite particle, while in \([2]\) it is positive as it describes a resonance in the continuum with a finite lifetime as evidenced by an imaginary contribution \([12]\) appearing in higher order terms in \( K \).

5. ABH-like mode solution of BS equations

The second solution of the coupled BS equation \([3]\) and \([4]\) follows from

\[
\begin{align*}
\frac{V k_F^2}{2\pi^2} & \int_{k_F - k_D}^{k_F + k_D} dk \int_{-1}^{1} dt v(|K/2 + k|) \times \\
& \times u(|K/2 - k|) u(|K/2 + k|) u(|K/2 - k|) + \\
& \times \varepsilon_K + E(|K/2 + k|) + E(|K/2 - k|) \times \\
& + \frac{V k_F^2}{2\pi^2} \int_{k_F - k_D}^{k_F + k_D} dk \int_{-1}^{1} dt u(|K/2 + k|) \times \\
& \times u(|K/2 - k|) u(|K/2 + k|) u(|K/2 - k|) + \\
& \times v(|K/2 + k|) v(|K/2 - k|) \times \\
& - \varepsilon_K + E(|K/2 + k|) + E(|K/2 - k|) = 1. \tag{14}
\end{align*}
\]

Proceeding as before, in the limit \( K \to 0 \) one now finds

\[
\varepsilon_K = (v_F hK/\sqrt{3})[1 + \frac{\hbar \omega_D}{4E_F} e^{-2/\lambda} + \cdots] + O(K^2), \tag{15}
\]

which is similar to the Anderson-Bogoliubov-Higgs (ABH) RPA excitation mode in the BCS theory of superconductivity \([10,13,13]\).

6. Conclusion

We have presented a new many-fermion formalism based on a BS equation applied to the full BCS ground state which does not neglect the presence of holes. This leads in the ladder approximation to two types of solutions: the first referring to simple moving CPs consisting of two-electron \((12)\) or two-hole \((13)\) resonances. In addition, this formalism naturally provides a second solution \((15)\) of an entirely different physical nature which is analogous to the ABH excitation mode. Bose-Einstein condensation can occur with the first type of objects but not with the second.

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