Cooper-pair size and binding energy for unconventional superconducting systems

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The main proposal of this paper is to analyze the size of the Cooper pairs composed by unbalanced mass fermions from different electronic bands along the BCS-BEC crossover and study the binding energy of the pairs. We are considering an interaction between fermions with different masses leading to an inter-band pairing. In addition to the attractive interaction we have an hybridization term to couple both bands, which in general acts unfavorable for the pairing between the electrons. We get first order phase transitions as the hybridization break the Cooper pairs for the shell-wave symmetry of the gap amplitude. The results show the dependence of the Cooper-pair size as a function of the hybridization for T = 0. We also propose the structure of the binding energy of the inter-band system as a function of the two-bands quasi-particle energies.

I. INTRODUCTION

The unconventional superconducting systems remain an open subject in the condensed matter physics. The pairing mechanism by which electrons are bound together to form pairs in these systems is one of the main issues. The superconducting (SC) state arises from electron pairing and the onset of long-range phase coherence where the phenomena may occur at different temperatures or other tuning parameters. For conventional SC materials the pairing arises indirectly by the exchange of phonons of the crystal lattice and shows a Cooper pair size around \( \xi \sim 10^3 - 10^4 \) Å. For the unconventional SC materials the superconducting pairing mechanism is not completely established. Their short Cooper pair size in comparison with conventional materials \( (\xi \sim 10^0 - 10^1 \) Å) have influenced theoreticians to introduce new hypotheses to explain the electron pairing via, for example, spin fluctuations and short-range spin waves [2].

The shell-wave single-band models are able to describe pure metallic superconductors, alloys and systems of cold atoms [3], where it is possible to study the superfluid ground state in all ranges of attractive interactions from the BCS scenario (weak coupling) to the Bose-Einstein Condensate (strong coupling). In the cold atoms case it is possible to observe in the strong coupling limit the occurrence of Bose-Einstein Condensate (BEC) that is obtained by the single-band model. However to study more complex systems like the heavy fermion metals, the single-band model is not enough to explain all the experimental features observed. The heavy fermion systems [4] have their peculiar properties related to the effects that the electrons show due to different electronic band widths. Thus, multi-band models are adopted to describe these compounds allowing the study of heavy-fermion superconductivity. These multi-band models are similar to that which was introduced by Suhl et al. [5], with the presence of a hybridization term between the bands, that can be tuned experimentally for example by external pressure.

For our case, we are interested to analyze the superconductivity for a system where the Cooper pairs are composed by fermions with different masses. For this purpose we introduce a two-band Hamiltonian where one band is related to a free electrons and the second one is composed by fermions with effective mass higher than the free electrons one. The two-band model Hamiltonian with hybridization is given by

\[
\mathcal{H} = \sum_{k,\sigma}(\varepsilon_k^a a_{k,\sigma}^\dagger a_{k,\sigma} + \varepsilon_k^b b_{k,\sigma}^\dagger b_{k,\sigma}) + V \sum_{k\sigma}(a_{k,\sigma}^\dagger b_{k,\sigma} + b_{k,\sigma}^\dagger a_{k,\sigma}) - U \sum_{kk'} a_{k,\sigma}^\dagger b_{-k',\sigma}^\dagger a_{-k',\sigma}, \tag{1}
\]

where \( a_{k,\sigma}^\dagger \) and \( b_{k,\sigma}^\dagger \) are creation operators for the light \( a \) and the heavy \( b \) quasi-particles, respectively, with two hyperfine states labeled as \( \sigma = \uparrow \) (up spin) or \( \downarrow \) (down spin). The energies \( \varepsilon_k^a,b = \sum_j t_{ij} e^{ik(r_i-r_j)} \) are the dispersion relation of each band with \( t_{ij} \) being the hopping amplitudes. \( V \) is the hybridization term and \( U \) is a local attractive potential among fermions from different bands. In general, the hybridization is used as a control parameter to explore the phase diagram, driving the system for the superconductor quantum critical points (SQCP) separating normal and superconducting phases.

II. THE GREEN’S FUNCTION OF SYSTEM

We have done the Hartree-Fock mean field approximation to decouple higher order Green’s functions generated by the equations of motion yielding a closed system of equations. The relevant wave-vector and frequency dependent Green’s functions are given by
<[a_k \sigma; a_{k,\sigma}^\dagger]> = \frac{W_{k,\sigma}^2 \Omega_{k,\sigma}^+ - \Delta_{ab} \Omega_{k,\sigma}^+ + V^2 \Omega_{k,\sigma}^-}{2\pi \rho(\omega)}, \tag{2}
\langle b_{k \sigma}^-; b_{k,\sigma}^\dagger \rangle = \frac{W_{k,\sigma}^2 \Omega_{k,\sigma}^- - \Delta_{ab} \Omega_{k,\sigma}^- - V^2 \Omega_{k,\sigma}^+}{2\pi \rho(\omega)}, \tag{3}

and
\langle b_{k,\sigma}^-; a_{k,\sigma}^\dagger \rangle = \frac{\Delta_{ab} (\Omega_{k,\sigma}^+ - V^2 - \Omega_{k,\sigma}^+ \Omega_{k,\sigma}^-)}{2\pi \rho(\omega)}. \tag{4}

where \( \Omega_{k,\sigma}^\pm = (\omega \pm \varepsilon_k^\pm, W_{k,\sigma}^\pm = (\omega^2 \pm \varepsilon_{2a,b}) \) and \( \rho(\omega) \) the polynomial
\[
P(\omega) = \omega^4 - \left[ \varepsilon_k^2 + \varepsilon_k^2 + 2(\Delta_{ab}^2 + V^2) \right] \omega^2 + \left[ \varepsilon_k^a \varepsilon_k^b - (V^2 - \Delta_{ab}^2) \right]. \tag{5}
\]

For this scenario \( \Delta_{ab} \) is the inter-band superconductor order parameter, given by:
\[
\Delta_{ab} = U \sum \langle a_{k,\sigma}^\dagger b_{k,\sigma}^\dagger - \sigma \rangle. \tag{6}
\]

We insert a simple notation to represent the inter-band pairing correlation functions as
\[
\phi_{ab}(k) = \langle a_{k,\sigma}^\dagger b_{k,\sigma}^\dagger \rangle. \tag{7}
\]

The anomalous Greens’s function calculated \( \langle b_{k,\sigma}^-; a_{k,\sigma}^\dagger \rangle \) allow one to obtain the correlation function previously described \( \phi_{ab}(k) \) through the Fluctuation-Dissipation Theorem as follows
\[
\phi_{ab}(k) = \int d\omega f_{FD}(\omega) \sum \langle b_{k,\sigma}^-; a_{k,\sigma}^\dagger \rangle, \tag{8}
\]
where \( f_{FD}(\omega) = [\exp(\beta \omega) + 1]^{-1} \) is the Fermi-Dirac function \( (\beta = 1/k_B T \) where \( k_B \) is the Boltzmann constant and \( T \) the temperature). After perform these calculations we get (for \( T = 0 \)):
\[
\phi_{ab}(k) = \frac{\Delta_{ab}}{2(\omega_{1k}^2 - \omega_{2k}^2)} \sum_{i=1}^2 (-1)^{i+1} \frac{\omega_{1k}^2 - \varepsilon_{k,i} \varepsilon_{k,i} - \Delta_{ab}^2 + V^2}{\omega_{1k}}. \tag{9}
\]

The roots of the polynomial \( P(\omega) \) in Eq. (5) yield the poles of the Green’s functions and determine the energy of the excitations of the two-band superconductor. These are given by:
\[
\omega_{1,2k} = \sqrt{A(k) \pm \sqrt{B(k)}}, \tag{10}
\]
with
\[
A(k) = \frac{\varepsilon_k^a + \varepsilon_k^b + 2(\Delta_{ab}^2 + V^2)}{2}.
\]

and
\[
B(k) = \left[ \frac{(\varepsilon_k^a - \varepsilon_k^b)^2}{2} + V^2 \right] \left[ (\varepsilon_k^a + \varepsilon_k^b)^2 \right] + \Delta_{ab}^2 \left[ (\varepsilon_k^a - \varepsilon_k^b)^2 + 4V^2 \right].
\]

In our analysis, we assume that the bands display the same shape being homotetic, i.e., \( \varepsilon_k^a = \alpha \varepsilon_k^b \) with \( \varepsilon_k^a = k^2/2m_a - \mu \) where \( \alpha \) is the ratio of the effective masses of the quasi-particles in the two bands given by \( \alpha = m_a/m_b \), with \( m_a \) and \( m_b \) being the masses of the particles of the wide and the narrow band, respectively. The chemical potential \( \mu \) is the same for both bands. Since the b-electrons from the narrow band are heavier, \( \alpha < 1 \). We consider the total number of electrons \( N = \sum_k \langle n_k \rangle + \langle n_k^b \rangle \) as fixed, where \( \langle n_k \rangle = \langle a_k^\dagger a_k \rangle \) and \( \langle n_k^b \rangle = \langle b_k^\dagger b_k \rangle \) are calculated similarly as done in Eq. (5) for the anomalous Green’s functions.

We now obtain the number and the gap equations for a three dimensional system with s-wave order parameter symmetry. These must be solved self-consistently. The number equation for \( T = 0 \) is obtained from the propagators (2) and (3). It is given by:
\[
N = \frac{k_B^2}{4\pi^2} \int_{-\gamma}^{\gamma} \sqrt{x + \mu} \left\{ \frac{1 - \frac{x}{2(\omega_{1x}^2 - \omega_{2x}^2)}}{2(\omega_{1x}^2 - \omega_{2x}^2)} \right\} \sum_{i=1}^2 (-1)^{i-1} \frac{\omega_{1x}^2 - \Delta_{ab}^2 + V^2 - \alpha x^2}{\omega_{1x}} \right\} dx, \tag{11}
\]
where \( \omega_{1,2x} \) are the excitation energies of the system given by (10). The sum over \( k \) was changed into an integral, and we introduced a dimensionless variable \( x \). The over-bar in a given quantity means that it is normalized by the Fermi energy \( E_F \).

In a pure inter-band scenario i.e., without any contribution of a intra-band attractive interaction, it is observed a first-order phase transition at low temperatures and a second-order phase transition for higher temperatures. In consequence, a tricritical point (TCP) in the phase diagram was found similar to that observed experimentally in superconducting systems with an applied magnetic field. However in our description we have no presence of a magnetic field, instead we have a control parameter, the hybridization, that can be tuned by external pressure or doping. In general these observations indicate the possibility of measuring discontinuities in the SC gap amplitude by applying pressure to the system.

In the Suhl model the hybridization between the bands was neglected but they included an “inter-band” term that creates (annihilates) an intra-band pair from one band and annihilates (creates) an intra-band pair from the other one. Thus the model that we adopted in this section is different because we do not consider any kind of intra-band pairs. Our attractive inter-band interaction creates a pair composed by quasi-particles from different
species as pointed out by V. Liu and F. Wilczek to propose a new state of matter in which the pairing interactions create a gap within the interior of a large Fermi ball, while the exterior surface remains gapless. In general, the pairing occurs between two species whose Fermi surfaces do not match simply because their densities or effective masses differ. This possibility arises in solids for example if the electron populations in the two bands are unbalanced.

The hybridization mechanism is responsible for the mixing among the quasi-particles from different bands. In metallic systems, such as transition metals, inter-metallic compounds and heavy fermions, this term arises from the mixing of the wave-functions of the quasi-particles in different orbitals through the crystal lattice potential. For another systems as the problem of color superconductivity, it is the weak interaction that allows the transformation between up and down-quarks. For a system of cold fermionic atoms in an optical lattice with two atomic states, the hybridization is related to Raman transitions with an effective Rabi frequency which is linearly proportional to . Then, the physical origin of the -term is different for each case. Nevertheless, the main point is that at least in inter-metallic systems, the hybridization can be easily controlled by pressure or doping, allowing one to explore their phase diagrams. That is one of the most interesting aspects that lead us to use the these quantities as external control parameters, and that can be used to find for some systems the superconducting quantum critical point (SCQP) related to a second-order phase transitions.

From the Eqs. and we write the inter-band gap equation for as

\[
\frac{1}{U} = \sum_k \frac{1}{2(\omega_{1k} - \omega_{2k})^2} \sum_{i=1}^{2} (-1)^{i+1} \frac{(\omega_{1k} - \varepsilon_{i} \bar{c}^a_k \bar{b}^a_k - \Delta_{ab}^2 + V^2)}{\omega_{1k}}.
\]

(12)

We are interested to solve the gap equation in and calculate the inter-band Cooper-pair size and to analyze the effects of on these pairs along all spectra of interactions. Therfore we perform the renormalization technique in the gap equation in Eq. to remove the divergence of the integral in the strong coupling limit as made in Ref.. The standard solution of this problem is to transfer this divergence to the -wave scattering length . This quantity can be positive (strong coupling) or negative (weak coupling), and diverges at the unitarity limit as the systems crosses over BCS to the BEC limit. The scattering length parameter allows one to describe all regimes of attractive interactions between the quasi-particles. Thus, after performing the renormalization procedure in Eq. we obtain

where in this representation, plays the role of a dimensionless coupling constant, and is the Fermi wave vector. Notice that the integral limits in Eq. are . Similarly to the intra-band case, when one obtains the weak coupling regime (BCS limit), while for the system reaches the strong coupling limit (BEC limit).

The inter-band pair size is obtained using the definition based on the calculation

\[
\langle \xi_p^{\text{inter}} \rangle^2 = \frac{\int d^3k \phi_{ab}^*(k) \nabla_k^2 \phi_{ab}(k)}{\int d^3k \phi_{ab}^*(k) \phi_{ab}(k)}.
\]

(14)

where the inter-band pair wave function is given by the Eq. .

### III. Results and Discussions

Now, the integral that results from Eq. is solved together with the number equation and the renormalized gap equation self-consistently.
In Fig. 2 (a) (upper graph) we plot the numerical result for \( k_F \xi_p^{\text{inter}} \) for several values of hybridization \( V \). We observe that for non-hybrid case the numerical solution for \( \xi_p^{\text{inter}} \) is quite similar as that obtained the intra-band case, being a monotonically decreasing function of the attraction and proportional to \( 1/\Delta_{ab} \), going from the exponentially large value in the BCS limit. The numerical data for \( \Delta_{ab} \) and were obtained from self-consistently solutions of integrals in Eq. (11) and Eq. (13). For hybrid case \( (V > 0) \) we observe that the curves are quite different from the intra-band scenario: For a fixed value of hybridization we must achieve a minimum strength in the attractive interaction to get a solution for the problem. For example, for \( V = 0.2 \) does not exist solutions for \( 1/k_F a_s < -1 \), i.e., for a fixed attractive interaction there is a characteristic value of hybridization which leads the system from a SC state to the normal one. This fact is related to the First-order transitions that occur in the inter-band scenario as observed in Ref. 22. From another point of view the attractive interaction must overcome the quantum barrier imposed by the hybridization, i.e. the superconducting state arises when \( \Delta_{ab} > V \). The First-order transition in the BCS-BEC crossover for the inter-band case was firstly pointed out in Ref. 22. Nevertheless the convergence observed only in the BEC limit for the intra-band case is now observed also in the BCS and BEC limits for inter-band case. In the BEC limit we observe a convergence of all solutions for different hybridization strength going to the same size of the two-body bound state observed for \( V = 0 \).

In the Fig. 2 (b) (lower graph) we plot \( k_F \xi_p^{\text{inter}} \) for several values of mass ratio \( \alpha \). In the BCS regime, for systems where \( \alpha \) is close to 1, as our result for \( \alpha = 0.8 \), the Cooper pair is composed by fermions with balanced masses as those found in conventional systems. The size of these pairs are much bigger than those formed by unbalanced masses as our result for \( \alpha = 0.2 \). The short size of the Cooper-pairs for the case where \( \alpha \) is small, it is comparable to the heavy fermions superconductors (HFSC) and the HTSC where \( \alpha \ll 1 \) and is in agreement with experimental observations. For conventional BCS SC materials the Cooper pair size is around \( \xi_p \sim 10^3 - 10^4 \) A, while for the unconventional SC materials the Cooper pair size is around \( \xi_p \sim 10^9 - 10^{10} \) A.

At this point it is possible to perform a comparison between intra-band and inter-band systems. In Fig. 3 we plot the results for \( \xi_p^{\text{intra}} \) and \( \xi_p^{\text{inter}} \) for non-hybrid \( V = 0 \) case. We observe that in the BCS limit the inter-band Cooper-pair is much bigger than the intra-band one. This fact corroborates with another theoretical observations. This fact indicates that for a same attractive interaction strength, the intra-band gap amplitude \( \Delta \) is bigger than \( \Delta_{ab} \). In the BCS-BEC crossover region \( (-1 < 1/k_F a_s < +1) \) we observe that close to the unitarity \( (1/k_F a_s = 0) \) both sizes coincide \( \xi_p^{\text{intra}} = \xi_p^{\text{inter}} \). In this region of attractive interactions a Cooper-pair composed of fermions with same mass has the same size of the other one composed of an unbalanced massive fermion system and \( \Delta \sim \Delta_{ab} \). This observation indicates that in the BCS-BEC crossover the \( \alpha \) factor (masses ratio) is not relevant to determine the Cooper-pair size for both kind of interaction (intra or inter-band). At this point for higher interactions there occurs a significant change in the major size of Cooper pairs. Now when the system is driven to the BEC limit, the inter-band Cooper-pair size becomes slightly smaller than the intra-band one, i.e., \( \Delta < \Delta_{ab} \). However this fact does not change the main feature of the system: the first-order phase transition of inter-band scenario.

In the Fig. 3 we analyze with more attention the inter-band Cooper-pair size dependence with hybridization \( V/E_F \) for several values of attractive interaction for BCS \( (1/k_F a_s < 0) \) and BEC limits \( (1/k_F a_s > 0) \). In this case the system behaves similarly as the for finite temperatures: generally the Cooper-pair size is independent of temperature for conventional superconductors. Our results show that \( \xi_p^{\text{inter}} \) is not modified by hybridization until the characteristic \( V \). When \( V \) reaches the condition \( V \geq \Delta_{ab} \) the inter-band Cooper pair is abruptly broken and is observed one of the most relevant features of inter-band superconductivity, the first-order phase transition. However the order of magnitude of \( k_F \xi_p^{\text{inter}} \) for both BCS and BEC limits is not altered in comparison to intra-band case: In the BCS limit where \( 1/k_F a_s < 0 \), \( k_F \xi_p^{\text{inter}} \sim 10^1 - 10^2 \). In BEC limit we observe that even for decades of order of magnitude for \( V \), \( \xi_p^{\text{intra}} \) keeps unaltered around \( k_F \xi_p^{\text{inter}} \sim 10^{-10} \).
In the strong coupling regime we get pair of fermionic quasi-particles with different masses.

Similarly to the intra-band case, the gap at \( k = 0 \) can be associated to the dissociation energy of the effective bosons formed now by the strongly coupled pairs of fermionic quasi-particles with different masses.

In the Fig. 3 we plot the energies \( \omega_1 \) and \( \omega_2 \) for \( k = 0 \) as a function of the attractive interaction. We are interested in observing the dissociation energy of the effective bosons of the system as a function of \( 1/k_F a_s \). For this inter-band scenario, in the weak coupling limit \( \alpha = 1 \), i.e., \( \omega_1 = E_F \) and \( \omega_2 = 0.5 \) as expected for the BCS limit.

In the Fig. 4 we plot the dispersion relations of the inter-band excitations \( \omega_1(k) \) and \( \omega_2(k) \) in the BCS weak coupling regime and the strong coupling BEC regime for \( V/E_F = 0.1 \) and \( \alpha = 0.5 \).

**A. Spectral analysis and the binding energy of system**

In this section we study the spectra of the system. From numerical data we can perform a spectral analysis of the quasi-particles \( \omega_1(k) \) and \( \omega_2(k) \) along the BCS-BEC crossover at \( T = 0 \). For the inter-band case for a fixed hybridization \( V/E_F = 0.1 \) we plot the results in Fig. 3. In the BCS limit (dotted lines) the typical dip close to the Fermi wave vector for \( \omega_1(k) \) and \( \omega_2(k) \) is observed. In this picture \( \Delta_{ab} \) reaches the minimal value to give rise the inter-band SC state. In the strong coupling case (full lines) shown in Fig. 4 the dispersion relations are similar to those observed in the intra-band case.

The effective Boson particles with a quadratic dispersion. In this case \( \Delta_{ab} > V \) and there are no gapless or dip point in the spectra. Similarly to intra-band case, the gap at \( k = 0 \) can be associated to the dissociation energy of the effective bosons which behaves like as free particles with a quadratic dispersion as shown in Fig. 4. Nevertheless, differently of the intra-band case where the binding energy was purely the \( \omega_2 \) that displays a dip for \( \mu = 0 \), for the inter-band case we found that the binding energy \( E_b \) of the system is written as the difference between both branches of energies, i.e., \( E_b = \omega_1 - \omega_2 \), that dip and reaches the minimum value when \( \mu = 0 \) (dotted vertical line) as shown in the Fig. 5. Notice that \( E_b \) does not display a dependence with the hybridization based on our result shown in Fig. 3. That is a remarkable feature and it is a significant difference in comparison with the intra-band system where \( E_b \) has a power law in function of \( V \). However \( E_b \) shows a dependency with the mass ratio \( \alpha \). A clear evidence is shown the Fig. 11 where for a fixed attractive interaction, the \( \xi_{inter} \) get higher as \( \alpha \) increases. Performing an expansion of \( E_b \) as a function of \( \alpha \) we get

\[
E_b(\alpha, \Delta_{ab}, \mu) = A_0 - A_1 \alpha + O(\alpha^2),
\]

where

\[
A_0(\Delta_{ab}, \mu) = \frac{A^+(\Delta_{ab}, \mu) - A^-(\Delta_{ab}, \mu)}{2}
\]

and

\[
A_1(\Delta_{ab}, \mu) = \frac{2\mu \Delta_{ab}^2}{\sqrt{\mu^2 + 4\Delta_{ab}^2}} \left( \frac{1}{A^+(\Delta_{ab}, \mu)} - \frac{1}{A^-(\Delta_{ab}, \mu)} \right),
\]

with the coefficients

\[
A^\pm(\Delta_{ab}, \mu) = \sqrt{2\mu^2 + 4\Delta_{ab}^2} \pm 2\mu \sqrt{\mu^2 + 4\Delta_{ab}^2}.
\]
FIG. 5: The energies $\omega_1$ and $\omega_2$ for $k = 0$ as a function of the attractive interaction in the BCS weak coupling regime and strong coupling BEC regime and the difference $(\omega_1 - \omega_2)/E_F$ for $V/E_F = 0.1$ and $\alpha = 0.5$.

We may notice that the Eq. (14) is suitable for a little \(\alpha\), where the term $O(\alpha^2)$ can be neglected. Also in the Eq. (15) we observe that while $\alpha$ increases $E_b$ linearly decreases.

IV. CONCLUSIONS

In this work, we have studied the effects of hybridization $V$ on the superconducting ground state and on the inter-band Cooper-pair size. We adopted the two-band model with an inter-band attractive interaction. Using the Hartree-Fock mean field approximation we obtain the normal and anomalous Green’s functions which are then used to determine the gap and number equations, and the Cooper-pair size equation. These equations are then solved self-consistently separately.

In order to observe the hybridization effects on Cooper-pair size for inter-band interactions and study all ranges of interactions (BCS weak coupling limit and the BEC strong coupling limit) we renormalized the gap equation, by introducing the scattering length for the two-band problem. For $V = 0$ the inter-band case shows the expected smooth evolution for $\xi_{\text{inter}}^b$ between weak and strong coupling limits. In the BEC limit we observe a convergence of all solutions for different hybridization strength going to the same size of the two-body bound state observed for $V = 0$. However for a fixed attractive interaction strength, $\xi_{\text{inter}}^b$ does not change and keep the same size until a certain value of $V$ where $\xi_{\text{inter}}^b$ suddenly disappears when the Cooper-pair is broken. These facts are related to the first-order transitions observed by the discontinuities in the inter-band gap amplitude $\Delta_{ab}$.

In the BEC limit we have observed that the difference between the quasi-particle energies $\omega_1 - \omega_2$ becomes the pair binding energy for $k = 0$. When the chemical potential goes to $\mu = 0$, it was observed the minimum in the binding energy where the superconducting ground state is now composed by the effective bosons. We also performed an expansion of the binding energy $E_b$ as a function of the mass ratio and was observed that while $\alpha$ increases $E_b$ decreases.

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