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# First and second order quantum phase transitions in multi-band superconductors

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In multi-band and inter-metallic materials superconductivity can be destroyed by applying external pressure in these systems. In many cases the critical temperature is driven continuously to zero, the superconducting to normal transition being associated with a superconducting quantum critical point (SQCP). In this paper we propose a model for this type of SQCP based on the increase of hybridization as pressure is applied in the material. We study a two-band superconductor with hybridization $V$ between these bands. We use a BCS approximation and include both inter- and intra-band attractive interactions. We show that for negligible inter-band interactions, as hybridization increases there is a second order phase transition from a superconductor to a normal state at zero temperature at a critical value of the hybridization $V_c$. This SQCP can be reached by pressure, since this external parameter controls hybridization in the system. We also find discontinuous transitions at zero temperature and the appearance of a gapless superconducting (GS) phase in a certain range of hybridization in the case of inter-band interactions being dominant.



## 1. Introduction

The study of asymmetric superconductivity, i.e., of superconductivity in systems with mismatched Fermi surfaces, has raised a lot of interest over the last years [1]. This in part is due to the relevance of this problem for many different areas in physics. Such a problem arises in cold atom systems with superfluid phases, color superconductivity in the core of neutron stars and condensed matter physics. Furthermore this problem is closely related to inhomogeneous superconductivity, as FFLO phases, since these are possible ground states for asymmetric systems. In condensed matter systems as inter-metallic materials there is natural mismatch in Fermi surfaces due to different bands of electrons occurring at the Fermi surface with different Fermi wave-vectors [2]. Then, even in the absence of external magnetic fields, one has to consider the possibility of inhomogeneous superconductivity or other types of exotic ground states as gapless superconducting (GS) phases. In this work we study asymmetric superconductivity in a two-component system with attractive interactions among the same and different components. This model is specially suited to describe two bands inter-metallic compounds [2]. For completeness we take into account hybridization among the different components, such that only the total number of particles is conserved.

In condensed matter, multi-band superconducting (SC) systems are susceptible to external pressure and in many cases this drives them to the normal metallic state through a superconducting quantum critical point (SQCP). There are few mechanisms that can produce this type of quantum phase transition. The most well known is through magnetic impurities [3], but there is no reason to expect that this should be important in systems which are brought to the normal state by external pressure. Here we propose an alternative mechanism which is due to the increase of hybridization caused by applying external pressure. In condensed matter, multi-band systems, pressure modifies the overlap of the wave-functions and consequently varies their hybridization. In this paper we study the different types of zero temperature superconductor to normal metal phase transitions that can occur in a multi-band system as hybridization (pressure) increases. We find that this transition can be discontinuous, but in the case of predominant inter-band interactions the superconductor–normal phase transition is of second order and occurs through a SQCP.

## 2. Model and formalism

We consider a model with two types of quasi-particles, $a$ and $b$, with an attractive inter-band interaction [4] $g$, an attractive intra-band interaction $U$ and a hybridization term $V$ that mixes different quasi-particles states [2]. This one-body mixing term $V$ can be tuned by external parameters such as pressure, permitting the

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exploration of the phase diagram and quantum phase transitions of the model. The Hamiltonian is given by

$$H=\sum_{k\sigma}\varepsilon_k^a a_{k\sigma}^\dagger a_{k\sigma}+\sum_{k\sigma}\varepsilon_k^b b_{k\sigma}^\dagger b_{k\sigma}+g\sum_{kk'\sigma}a_{k'\sigma}^\dagger b_{-k'-\sigma}^\dagger b_{-k-\sigma}a_{k\sigma}+U\sum_{kk'\sigma}b_{k'\sigma}^\dagger b_{-k'-\sigma}^\dagger b_{-k-\sigma}b_{k\sigma}+\sum_{k\sigma}V_k(a_{k'\sigma}^\dagger b_{k\sigma}+b_{k\sigma}^\dagger a_{k\sigma}) \quad (1)$$

where $a_{k\sigma}^\dagger$ and $b_{k\sigma}^\dagger$ are creation operators for the light $a$ and the heavy $b$ quasi-particles, respectively. The dispersion relations $\varepsilon_k^a = k^2-1$ and $\varepsilon_k^b=\alpha k^2-b$ with the ratio between effective masses is taken as $\alpha=(m_a/m_b)$.

The $V$-term is responsible for the transmutation among the quasi-particles. In metallic systems, as transition metals [5], intermetallic compounds and heavy fermions [6], it stems from the mixing of the wave-functions of the quasi-particles through the crystalline potential. In the quark problem, it is the weak interaction that allows the transformation between up and down-quarks and gives rise to the mixing term [1,7,8]. For a system of cold fermionic atoms in an optical lattice, with two atomic states ($a$ and $b$), the $V$-term is due to Raman transitions with an effective Rabi frequency which is directly proportional to $V$ [9]. Thus, the hybridization term is added to take into account these effects that allow for a quasi-particle ($a$ or $b$) transform into one another, so that only the total number of particles ($a+b$) is conserved. The physical source of the $V$-term is different for each of the systems, as described previously. In the metallic case, which is our principal interest here, hybridization can be easily controlled by applied pressure that varies the overlap between the atomic wave-functions. It provides this way a very useful control parameter that can be changed externally, allowing to probe experimentally the phase diagram of these materials.

Since we know the form of the Hamiltonian that we want to study, we can, respectively, write the superconducting order parameters, asymmetrical and symmetrical of the system, such as $\Delta_{ab}=-g\sum_{k\sigma}\langle b_{-k-\sigma};a_{k\sigma}\rangle$ and $\Delta=-U\sum_{k\sigma}\langle b_{-k-\sigma};b_{k\sigma}\rangle$, respectively.

In order to obtain the spectrum of excitations of Eq. (1) within the mean-field approach, we use the equation of motion method to calculate standard and anomalous Greens functions [10]. Excitonic types of correlations that just renormalize the hybridization [11] have been discarded. For the purpose of obtaining the order parameters, the anomalous Greens function is necessary to be calculated, $\langle\langle a_{k\sigma};b_{-k-\sigma}\rangle\rangle$ and $\langle\langle b_{k\sigma};b_{-k-\sigma}\rangle\rangle$. When we write the equation of motion for these Greens functions, new Greens functions are generated [10]. Some of these are of higher order as they contain a larger number of creation and annihilation operators than just the two of the initial Greens functions. For these, we apply a BCS type of decoupling [10] to reduce them to the order of the original propagators. Finally, writing the equations of motion for the new Greens functions, we obtain a closed system of equations that can be solved as we did before [2].

From the discontinuity of the Greens functions on the real axis we can obtain the anomalous correlation function characterizing the superconducting state. For the frequency of these excitations to vanish, it is required that $[\varepsilon_k^a\varepsilon_k^b-(V^2-\Delta_{ab}^2)]^2+\Delta^2\varepsilon_k^{a2}=0$. This can occur by tuning the hybridization parameter, such that $V=\Delta_{ab}$ in which case gapless excitations appear at $k=k_F^a$ where $\varepsilon_k^a=0$. Without this fine tuning there are no gapless modes. Yet this does not occur if the symmetric interaction is zero, because in that case the frequency of excitations could vanish if $\varepsilon_k^a\varepsilon_k^b-\left(V^2-\Delta_{ab}^2\right)=0$, we will see the effects of this behavior in the next section of this paper. For symmetry reasons, we obtain the energy of the excitations in the form $\omega_{1,2}=\sqrt{A_k\pm\sqrt{B_k}}$ with

$$A_k=\frac{\varepsilon_k^{a2}+\varepsilon_k^{b2}}{2}+\Delta_{ab}^2+V^2+\frac{\Delta^2}{2} \quad (2)$$

and

$$B_k=\left(\frac{\varepsilon_k^{a2}-\varepsilon_k^{b2}}{2}\right)^2+V^2(\varepsilon_k^a+\varepsilon_k^b)^2+\Delta_{ab}^2(\varepsilon_k^a-\varepsilon_k^b)^2+4V^2\Delta_{ab}^2+\frac{\Delta^4}{4}-\frac{\Delta^2}{2}(\varepsilon_k^{a2}-\varepsilon_k^{b2})+\Delta^2(V^2+\Delta_{ab}^2) \quad (3)$$

The order parameters are determined by two coupled equations which for finite temperature are given by

$$\frac{1}{g\rho}=\sum_{j=1}^{2}\int_{-\omega_D}^{\omega_D}\frac{d\varepsilon}{2\sqrt{B(\varepsilon)}}\left[(-1)^j\Phi(\varepsilon)\tanh\left(\frac{\beta\omega_j(\varepsilon)}{2}\right)\right] \quad (4)$$

with

$$\Phi(\varepsilon)=\left(\frac{\omega_j^2(\varepsilon)-\gamma^2(\varepsilon)}{2\omega_j(\varepsilon)}\right) \quad (5)$$

$$\gamma^2(\varepsilon)=\left[\frac{\varepsilon+(\alpha\varepsilon-b)}{2}\right]^2+(\Delta_{ab}^2-V^2)+\frac{\Delta V}{4}\left[\Delta V+4\left(\frac{\varepsilon+(\alpha\varepsilon-b)}{2}\right)\right]-\left[\frac{\varepsilon+(\alpha\varepsilon-b)}{2}-\frac{\Delta V}{2}\right]^2 \quad (6)$$

with $\varepsilon_k^a=\varepsilon$, $\varepsilon_k^b=\alpha+(\alpha\varepsilon-b)$ and

$$\frac{1}{U\rho_b}=\sum_{j=1}^{2}\int_{-\omega_D}^{\omega_D}\frac{d\varepsilon}{2\sqrt{B(\varepsilon)}}\left[(-1)^j\Psi(\varepsilon)\tanh\left(\frac{\beta\omega_j(\varepsilon)}{2}\right)\right] \quad (7)$$

with

$$\Psi(\varepsilon)=\left(\frac{\alpha^2\omega_j^2(\varepsilon)-(\varepsilon+b-\alpha)^2}{2\alpha^2\omega_j(\varepsilon)}\right) \quad (8)$$

with $\varepsilon_k^a=(\varepsilon+b-\alpha)/\alpha$ and $\varepsilon_k^b=\varepsilon$.

The right-hand sides of Eqs. (4) and (7) define the gap functions $f(\Delta_{ab},\Delta)$ and $f_b(\Delta_{ab},\Delta)$, respectively. The behavior of gap function, free energy and phase diagrams for null temperature of the system, will be graphically analyzed in the next section.

## 3. Results and discussions

### 3.1. Pure asymmetrical case ($\Delta=0$) at $T=0$

We will, at first, analyze the case with $T=0$. Considering the case with only the inter-band term (asymmetrical superconductivity) we observe that, the Hamiltonian which describes the model, we can get the thermodynamic properties of the system, one of them is the energy, as follows.

In Fig. 1 we show the energy of the ground state as a function of the order parameter for several values of the hybridization. We neglect the intra-band interaction and take the inter-band term as fixed while we vary the mixing $V$. These curves allow us to identify three characteristic values of hybridization. Initially for $V=V_1$ we notice the appearance of a minimum at the origin that coexists with the absolute minimum associated with the superconducting state. As hybridization increases, a first order phase transition at $V=V_2$ occurs, for which the energies of the normal and superconducting state are equal. Further increasing the hybridization, the superconducting state remains as a metastable state until $V=V_3$ where it stops being a minimum of the energy. These values of $V$ give rise to phase diagram that is shown in Fig. 2.

We clearly see in Fig. 2 the regions where the system presents its different behaviors. As explained before, for values $V>V_3$ the system is in the normal state (N) of conductivity. For $V_2<V<V_3$