Two-bands superconductivity with intra- and interband pairing for synthetic superlattices

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We consider a model for superconductivity in a two-band superconductor, having an anisotropic electronic structure made of two partially overlapping bands with a first hole-like and a second electron-like fermi surface. In this pairing scenario, driven by the interplay between interband V₁,₂ and intraband V₁,₁, pairing terms, we have solved the two gap equations at the critical temperature T = Tc and calculate Tc and the chemical potential µ as a function of the number of carriers n for various values of pairing interactions, V₁,₁, V₁,₂, and V₁,₂. The results show the complexity of the physics of condensates with multiple order parameters with the chemical potential near band edges.

I. INTRODUCTION

In a metallic system where both a first band V₁ and a second band V₂, with no hybridization, cross the Fermi level the pairing is described by a matrix where the diagonal elements are the intraband Cooper pairing processes, namely, V₁,₁ and V₂,₂ and the non-diagonal elements, namely, V₁,₂ that describes the interband pairing process associated with the transfer of pairs between the bands [1,3].

Today the open problem in condensed matter physics is the interband pairing where the standard BCS approximation that considers the Fermi level far away form the energy of band edges or critical points breaks down. In fact where the chemical potential is tuned near an electronic topological transition the high temperature superconductivity has been associated with quantum interference effects, called shape resonances, in the interband pairing terms since 1993 [4,5].

The shape resonance in the superconducting gaps is realized by material design of superconducting hetero-structures at atomic limit made of superlattices of superconducting layers with a relevant transversal hopping between layers [6,7]. The material architecture and the superlattice misfit strain [8,9] are key terms for fine tuning the system to quantum critical points [10,11] driven by electronic topological transitions.

At the time of discovery of high Tc cuprates in 1986, these materials have been considered to be isotropic 3D perovskites but later it was recognized that all high temperature superconducting cuprates are made of a superlattice of atomic copper oxide layers intercalated by different spacers where the evolution of the complex electronic structure with chemical doping has remained mysterious for many years. The large majority of scientific community has interpreted the available unconventional experimental data in terms of an effective single band for high temperature superconducting models. Few authors have interpreted the data in terms of mainly two non-hybridized bands and two Fermi surfaces at the nodal and anti-nodal point of the band structure [6,12]. This key point for the physics of cuprates has been recently accepted by the large scientific community in 2010 driven by compelling experimental data [13].

Later different practical realizations of superlattices of superconducting atomic layers intercalated by spacers tuned at a shape resonance [6] have been found in 2001 in diborides [15,30] and in 2008 in pnictides [31,33].

In these hetero-structures many experiments have provided experimental tests for multigap superconductivity in the clean limit also in the recognition of many lattice impurities introduced to change the chemical potential and structural phase separation from nano-scale to micron-scale [34,35] with the signatures of complexity of condensed matter near a quantum critical point. The key point for high temperature superconductivity is the presence of shape resonances in the interband pairing due to pair transfer between condensates with different topological symmetry due to quantum interference effects between pairing channel. This scenario has been discussed using simple electronic models [37,38].

Superconducting pnictides [31] are made of stacks of iron fcc atomic layers intercalated by spacers with a superlattice architecture similar to cuprates [7] that show multigap superconductivity [33] with multiple bands crossing the Fermi level [32].

While in diborides anomalous strong electron-phonon intraband interaction is quite relevant in two-band superconductivity scenario, in pnictides the intraband coupling is so small that has been neglected [33]. In fact experimental findings show that the scenario where interband pairing is the dominant interaction, proposed by some of us in previous works [39,40], has now an experimental test.
Here we investigate the case where the relative strength between the intraband and interband coupling is changing that is relevant for material design of novel high Tc superconductors made of synthetic superlattices. In this systems the relevant region for high temperature superconductivity is where the chemical potential is tuned between the band edge of the second band and the electronic topological transition where the Fermi surface of the second band changes from a 3D topology to a 2D topology with a corrugated cylindrical shape \[13\] \[14\]. Therefore we focus in a system with two similar overlapping bands such that the first hole-like (electron-like) Fermi surface coexists with a second electron-like (hole-like) Fermi surface.

The proposed model has the characteristic feature that for the occupation number of 1 electron per spin shows a critical point where the hole Fermi surface is the same as the electron Fermi surface (like in pnictides \[33\]) therefore tuning the chemical potential at this point there is a strong nesting between the two Fermi surfaces that determines a structural instability with a structural phase transition from tetragonal to orthorhombic phase \[10\]. A scale invariant complex structure could appear in the proximity of this phase transition in pnictides \[10\] as in cuprates \[34\].

We study a band structure that can be realized in superlattices of fcc lattice like in iron based multilayer materials that have provided a particular realization of multiband superconductivity in the clean limit with a high critical temperature.

In this paper we adopt the point of view that both the interband and intraband scattering terms are indeed very important to explain the response of the superconducting phase to the variation of the chemical potential. On the other side the case of pnictides is considered to be the case where intraband coupling can be neglected as we have proposed in the previous work before the discovery of pnictides \[40\]. Now we focus our interest on the fact that it is important to consider different cases where both intra-band and interband pairing are relevant that will be relevant for novel synthetic superconducting superlattices. We consider the case where the interband pairing \(V_{1.1}\) is as important as the intraband contributions, namely, \(V_{2.2}, V_{1.2}\). Here we report the study of the variations of the critical temperature and gap ratio as a function of the charge density crossing electronic phase transitions.

This paper is organized as follows. In Section II we present the four self-consistent equations: (1) two self-consistent equations (Eqs. (6 - 7)) to be solved at \(T = T_c\), namely, the equation for the superconducting critical temperature \(T_c\) coupled to the equation of the chemical potential \(\mu\) at a given particle density \(n\), and (2) three self-consistent equations for the gap parameters at \(T = 0\) and the total density (Eqs. (14 - 15)). In Section III we present our numerical results. Finally we conclude in Section IV.

II. THE EFFECTIVE HAMILTONIAN AND THE BCS EQUATIONS

The model Hamiltonian we use is the following

\[
H - \mu N = \sum_{k,\gamma} \varepsilon_1(\vec{k}) a_{\vec{k},\gamma}^\dagger a_{\vec{k},\gamma} + \sum_{k,\gamma} \varepsilon_2(\vec{k}) b_{\vec{k},\gamma}^\dagger b_{\vec{k},\gamma} \\
- V_{1.2} \sum_{\vec{k},\vec{k}'} \left[ a_{\vec{k},\uparrow}^\dagger a_{-\vec{k}',\downarrow} b_{\vec{k}',\uparrow} b_{-\vec{k}',\downarrow} + h.c. \right] \\
- V_{1.1} \sum_{\vec{k},\vec{k}'} \left[ a_{\vec{k},\uparrow}^\dagger a_{-\vec{k}',\downarrow} a_{\vec{k}',\uparrow} a_{-\vec{k}',\downarrow} \right] \\
- V_{2.2} \sum_{\vec{k},\vec{k}'} \left[ b_{\vec{k},\uparrow}^\dagger b_{-\vec{k}',\downarrow} b_{\vec{k}',\uparrow} b_{-\vec{k}',\downarrow} \right]
\]

(1)

where \(\gamma = \pm = \uparrow, \downarrow\) and

\[
\varepsilon_1(\vec{k}) = \varepsilon_1(\vec{k}) - \mu \\
\varepsilon_2(\vec{k}) = \varepsilon_2(\vec{k}) - \mu
\]

(2)

(3)

are the three-dimensional tight-binding bands of bands 1 and 2. In previous papers \[39\] \[40\], we have considered a Hamiltonian with \(V_{1.2} = V\), and \(V_{1.1} = V_{2.2} = 0\), as the interband and intraband pairing potentials, respectively. Here, these conditions are relaxed. We consider the simple case of a cubic lattice\[42\]. The energy band dispersion is given by

\[
\varepsilon_1(\vec{k}) = \varepsilon_1^0 - 2t_1 \left[ \cos(k_x) + \cos(k_y) + s_1 \cos(k_z) \right] \\
\varepsilon_2(\vec{k}) = \varepsilon_2^0 - 2t_2 \left[ \cos(k_x) + \cos(k_y) + s_2 \cos(k_z) \right].
\]

(4)

(5)
The Hamiltonian given in Eq. (1) is the same used in Ref. [39].

Going through the same technical steps followed in Ref. [39] we obtain the following self-consistent equations

\[ 1 - n = F_1(\mu, T_c) \]
\[ 1 = F_2(\mu, T_c, \omega_c) \]

where

\[ F_1(\mu, T_c) = F_{1,1}(\mu, T_c) + F_{1,2}(\mu, T_c) \]
\[ F_2(\mu, T_c, \omega_c) = [V_{1,2}^2 - V_{1,1}V_{2,2}] F_1 F_2 + V_{1,1} F_1 + V_{2,2} F_2 \]

and

\[ F_{1,1}(\mu, T_c) = \int_0^\pi \frac{d\vec{k}}{2 \pi^3} \tanh \left( \frac{\varepsilon_{1}(\vec{k})}{2k_B T_c} \right) \]
\[ F_{1,2}(\mu, T_c) = \int_0^\pi \frac{d\vec{k}}{2 \pi^3} \tanh \left( \frac{\varepsilon_{2}(\vec{k})}{2k_B T_c} \right) \]
\[ F_1 = \int_0^\pi \frac{d^3 \vec{k}}{2 \pi^3} \chi_{1}(\vec{k}) \tanh \left( \frac{\varepsilon_{1}(\vec{k})}{2k_B T_c} \right) \]
\[ F_2 = \int_0^\pi \frac{d^3 \vec{k}}{2 \pi^3} \chi_{2}(\vec{k}) \tanh \left( \frac{\varepsilon_{2}(\vec{k})}{2k_B T_c} \right) \]

where \( k_B \) is the Boltzmann constant and \( \chi_{i}(\vec{k}) = 1 \) if \( |\varepsilon_{i}(\vec{k})| \leq \omega_c \) and zero otherwise, \( i = 1, 2 \) and \( \omega_c \) is an energy cutoff (the Debye frequency) for the effective interaction. We solve the BCS equations at \( T = 0 \) K. These equations are:

\[ n = 1 - F_1'(\mu) \]
\[ \Delta_1 = \Delta_1^* G_1 \]
\[ \Delta_2 = \Delta_2^* G_2 \]

where

\[ F_1'(\mu) = \int_0^\pi \frac{d\vec{k}}{2 \pi^3} \left[ \frac{\varepsilon_{1}(\vec{k})}{E_1(\vec{k})} + \frac{\varepsilon_{2}(\vec{k})}{E_2(\vec{k})} \right] \]
\[ G_i = \int_0^\pi \frac{d\vec{k}}{2 \pi^3} \frac{\chi_{i}(\vec{k})}{E_i(\vec{k})} ; \quad i = 1, 2 \]
\[ E_i(\vec{k}) = \sqrt{\varepsilon_i(\vec{k})^2 + (\Delta_i^*)^2} ; \quad i = 1, 2 \]
\[ \Delta_1^* = V_{1,1} \Delta_1 + V_{1,2} \Delta_2 \]
\[ \Delta_2^* = V_{1,2} \Delta_1 + V_{2,2} \Delta_2 \]

Results for the numerical solution of the self-consistent Eqs. (6-15) are presented in Section III.

III. SEARCHING FOR SUITABLE PAIRING PARAMETERS AND NUMERICAL RESULTS

In Fig. 1 the two density of states \( N_1 \) and \( N_2 \), corresponding to the energy dispersion of Eqs. (2-3) are presented in panel (a) as a function of the electron number density per spin \( n \) for the band structure parameters chosen as \( t_1 = t_2 = 1 \) eV, \( s_1 = s_2 = 0.5 \), \( \epsilon_1^0 = 0.0 \) eV and \( \epsilon_2^0 = 4.5 \) eV, i.e., two similar overlapping bands so that the first hole-like (electron-like) Fermi surface coexists with a second electron-like (hole-like) Fermi surface.
The region where the interband pairing is relevant is shown in panel (b) of Fig. 1 (for $V_{1,1} = V_{2,2}$ and $V_{1,2}/V_{1,1} = 0.0, 0.5, 1.0, 1.5$ and $2.0$) by an effective density tracer given by the ratio $r(n) = V_{12} \sqrt{N_1 N_2} / \lambda_\perp$ where $\lambda_\perp$ is the effective density of states given by the standard BCS theory as:

$$T_c = 1.13 \ \omega_c \exp(\lambda_\perp)$$

where

$$\lambda_\pm = \frac{2 N_1 N_2 [V_{1,1} V_{2,2} - V_{1,2}^2]}{N_1 V_{1,1} + N_2 V_{2,2} \pm N}$$

$$N = \sqrt{|N_1 V_{1,1} - N_2 V_{2,2}|^2 + 4 N_1 N_2 V_{1,2}^2}.$$ 

Finally, in panel (c) of Fig. 1 we present the self-consistent numerical solution of Eqs. (14 -16) for the energy gap ratio $\Delta_2/\Delta_1$ for $T = 0 K$ in panel (a) and the self-consistent numerical solution of Eqs. (6-7) for $T_c \times n$ at $T = T_c$ in panel (b). For these plots we have chosen $V_{1,1}/t = V_{2,2}/t = 0.50$, $\omega_c/t = 1.00$ and $V_{1,2}/t = 0.375, 0.750, 1.125, 1.500$ and $1.875$.

IV. CONCLUSIONS

We have provided a theoretical description for multiband superconductivity in novel synthetic superlattices of superconducting layers with cubic lattice structure that will be essential for material design of possible room temperature superconductors [38]. We have investigated the two band superconductivity scenario for a two band superconducting layers with cubic lattice structure that will be essential for material design of possible room temperature superconductors [6, 38]. We have investigated the two band superconductivity scenario for a two band superconducting layers with cubic lattice structure that will be essential for material design of possible room temperature superconductors [6, 38].

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[1] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. 3, 552 (1969).
[2] J. Kondo, Prog. Theor. Phys. 29, 1 (1963).
[3] A. J. Leggett, Prog. Theor. Phys. 36, 901 (1966).
[4] A. Bianconi, Solid State Communications 89, 933 (1994), ISSN 00381098, URL \url{http://dx.doi.org/10.1016/0038-1098(94)90354-9}.
[5] For a review on multigap superconductivity and shape resonances: A. Bianconi, Journal of Superconductivity and Novel Magnetism 18, 25 (2005), ISSN 1557-1939, URL \url{http://dx.doi.org/10.1007/s10948-005-0047-5}.
In this paper, we follow the band structure of Eq. (4) that is appropriate for a generic cubic lattice like for the families of iron pnictides and for quantum size effects in superlattices made of layers with cubic structure. The band structure for the
MgB$_2$ hexagonal lattice (in 3-D) is given by

$$E_{1,2}(\vec{k}) = \pm V_1 \left( A(\vec{k}) + B(\vec{k}) \right)^{1/2}$$
\[+ 4 V_2 \cos(k_x a/2) \cos(\sqrt{3} k_y a/2)\]
\[+ 2 V_3 \cos(k_z c)\]

$$A(\vec{k}) \equiv \left[ \cos(k_y a/\sqrt{3}) + 2 \cos(k_y a/(2\sqrt{3})) \cos(k_z a/2) \right]^2$$

$$B(\vec{k}) + \left[ 2 \sin(k_y a/(2\sqrt{3})) \cos(k_z a/2) - \sin(k_y a/\sqrt{3}) \right]^2$$

where $V_{1,2}$ is the hopping integral between atoms placed on the hexagonal lattice (second type of atoms placed inside the primitive cell). $V_3$ is the effective hopping integral along the $c$–axis (or $z$–axis). The hexagonal lattice (Eq. 21) is left for a future calculation.
FIG. 1: Panel (a): the density of states $N_1$ and $N_2$ as a function of the carrier number $n$ according to the chosen band parameters $t_1 = t_2 = 1$ eV, $s_1 = s_2 = 0.5$, $\epsilon_0^1 = 0.0$ eV and $\epsilon_0^2 = 4.5$ eV; panel (b): the ratio $r(n) = V_{12} \sqrt{N_1 N_2 / \lambda}$ for $V_{1,1} = V_{2,2}$ and $V_{1,2} / V_{1,1} = 0.0, 0.5, 1.0, 1.5$ and 2.0 (see Eq. 20 for the definition of $\lambda$), useful as a tracer of the region where the interband pairing is relevant; panel (c): the self-consistent numerical solution of Eqs. (6-7) for chemical potential $\mu$ as a function of $n$ at $T = T_c$, which proved to be independent of the choice of $V_{1,1}, V_{2,2}, V_{1,2}$ and $\omega_c$ and matches to the $\mu \times n$ relation at $T = 0$ K obtained from Eqs. (14-16) (coloured online).
FIG. 2: For the given set of values $V_{11}/t = 0.50$, $V_{22}/t = 0.50$, $\omega_c/t = 1.00$, and $V_{1,2}/t = 0.375, 0.750, 1.125, 1.500, 1.875$ the panel (a) shows the self-consistent numerical solution of Eqs. (14-16) for the energy gap ratio $\Delta_2/\Delta_1$ at $T = 0 \text{K}$ and panel (b) shows the self-consistent numerical solution of Eqs. (6-7) for $T_c \times n$ at $T = T_c$. The solution of $T_c \times n$ for $V_{1,2}/t = 0.375$ is not shown in panel (b) since the values for $T_c$ in this case are too close to zero (coloured online).