Interorbital pairs in clean and impure superconductors

Anna Ciechan and Karol I Wysokiński
Institute of Physics and Nanotechnology Centre, M. Curie-Skłodowska University, ul. Radziwiłłowskiego 10, Pl 20-031 Lublin, Poland
E-mail: ankie@kft.umcs.lublin.pl (AC), karol@tytan.umcs.lublin.pl (KIW)

Abstract. We consider two orbital superconductor with spin singlet inter-orbital pairs only. The calculations of the local and global properties of such superconductor have been presented with special attention to the features which distinguish such system from the typical BCS one. In particular, in clean system we have found the existence of critical interaction $U$ necessary to induce superconducting transition and the asymmetry (with respect to the chemical potential) in the partial density of states. In the disordered system, in which the characteristics change from place to place, we have calculated local densities of states $N(\vec{r}, E)$ and local values of the order parameters $\Delta(\vec{r})$. Both $N(\vec{r}, E)$ and $\Delta(\vec{r})$ can be measured with help of scanning tunneling microscope.

1. Introduction
Materials with many bands near the Fermi energy offer a number of possible scenarios for the exotic quantum superconducting state. Despite the typical symmetries related to spin degrees of freedom we have new ones related to orbital quantum numbers. The discoveries of superconducting cuprates [1] and even more strontium ruthenate [2], magnesium diboride [3] and iron pnictides [4] have all greatly contributed to the development of the many band theory of superconductivity. Theoretical studies of superconductors with “overlapping bands” have been started by Suhl, Matthias and Walker and independently by Moskalenko in fifties [5] and were later continued by many others [6]. The understanding of many interesting properties of the above systems require new superconducting states. A good example are iron pnictides, which seem to be dominated by the inter band pairing scenario leading to the so called $s^{\pm}$ symmetry state characterized by constant gaps $\Delta_1, \Delta_2$ on two sheets of the Fermi surface, which for identical bands differ in sign ($\Delta_1 = -\Delta_2$) only [7, 8].

Of particular interest are the scenarios of superconductivity which rely on the unconventional spin or orbital symmetries. As an example let us mention the inter band superconductors. They are defined by the only (many particle) pairing interaction having, in the band picture, the form

$$H_{int} = U^{12} \sum_{\vec{k}, \vec{k}'} \left[ c_{1,\vec{k},\uparrow}^\dagger c_{1,\vec{k},\downarrow}^\dagger c_{2,\vec{k}',\downarrow} c_{2,\vec{k}',\uparrow} + c_{2,\vec{k},\downarrow}^\dagger c_{2,\vec{k},\uparrow}^\dagger c_{1,\vec{k}',\downarrow} c_{1,\vec{k}',\uparrow} \right].$$  \hspace{1cm} (1)

The Hamiltonian (1) describes the scattering of intra-band Cooper pairs and does not allow for inter-band pairs. In this work we are interested in the opposite situation and study the properties of two orbital superconductor with inter-orbital pairs. It means we consider the Cooper pairs...
in which each member belongs to different orbital. We shall call them superconductors with inter-orbital pairs. The properties of such systems markedly differ from the properties of inter-orbital superconductors or standard two-orbital superconductors with intra-orbital pairs. Similar models have earlier been considered in the context of photoinduced superconductivity in semiconductors [10], high temperature superconductors [11], cold atoms or quantum chromodynamic superfluids [12]. Recently superconductors with inter band pairs have been studied in the context of iron pnictides [13] and heavy fermions superconductors [14].

2. The model for two orbital superconductors

We consider the metallic system described by the two-orbital tight-binding model. The orbital description is especially important as we are also interested in the real space properties of the model. We consider the square lattice with two orbitals in each site. We assume the site dependence of parameters. The Hamiltonian reads

$$H = \sum_{ij,\lambda\lambda',\sigma} \left[ (e_{\lambda} - \mu) \delta_{ij} \delta_{\lambda\lambda'} - t_{ij}^{\lambda\lambda'} + V_{imp}(\vec{r}_j) \delta_{ij} \right] c_{i\lambda\sigma}^+ c_{j\lambda'\sigma}$$

$$- \sum_i U(\vec{r}_i)(c_{i1\uparrow}^+ c_{i2\downarrow}^+ + c_{i2\uparrow}^+ c_{i1\downarrow}^+)(c_{i1\downarrow} c_{i2\uparrow} + c_{i2\downarrow} c_{i1\uparrow}),$$

where $c_{i\lambda\sigma}$, $c_{j\lambda'\sigma}$ are the creation and annihilation operators of electrons with spin $\sigma = \uparrow, \downarrow$ at the lattice site $\vec{r}_i = i$ in the orbital $\lambda$, $e_{\lambda}$ is the electron on-site energy and $\mu$ the chemical potential. $t_{ij}^{\lambda\lambda'}$ are the hopping integrals between the same or different orbitals (if $\lambda \neq \lambda'$). $U(\vec{r}_i)$ denotes the attractive interactions responsible for inter-orbital pairing. They are allowed to vary from site to site in impure system. For such systems we also introduce local potential $V_{imp}^{\lambda\lambda'}$ at impurity sites $\vec{r}_i = i$ scattering electrons between two orbitals for $\lambda \neq \lambda'$. We limit our discussion to inter-orbital pairing scattering as it is expected to more severely affect the superconducting state with inter-orbital pairs in comparison to intra-orbital scatterers $V_{imp}^{\lambda\lambda'}$.

We use the standard mean-field decoupling valid for a spin singlet superconductor and get the effective Hamiltonian

$$H^{MF,A} = \sum_{ij,\lambda\lambda',\sigma} \left[ (e_{\lambda} - \mu) \delta_{ij} \delta_{\lambda\lambda'} - t_{ij}^{\lambda\lambda'} + V_{imp}(\vec{r}_j) \delta_{ij} \right] c_{i\lambda\sigma}^+ c_{j\lambda'\sigma}$$

$$+ \sum_{i,\lambda \neq \lambda'} \left[ \Delta(\vec{r}_i) c_{i\lambda\sigma}^+ c_{i\lambda'\sigma} + h.c. \right],$$

where the order parameters $\Delta(\vec{r}_i)$ are related to the pairing correlation functions through

$$\Delta(\vec{r}_i) = U(\vec{r}_i)(<c_{i1\downarrow} c_{i2\uparrow} > + <c_{i2\downarrow} c_{i1\uparrow} >).$$

Here we ignore Hartree terms $V_{\lambda\sigma}(\vec{r}_i) = U(\vec{r}_i)n_{\lambda'\sigma}(\vec{r}_i)(1 - \delta_{\lambda\lambda'})$, which depend on the number of particles at a given site $n_{\lambda\sigma}(\vec{r}_i) = <c_{i\lambda\sigma}^+ c_{i\lambda\sigma} >$.

The Hamiltonian (3) is diagonalized by means of the Bogoliubov - Valatin transformation [15]

$$c_{i\lambda\uparrow} = \sum_{\nu} \left[ u_{\lambda\nu}(\vec{r}_i) \gamma_{\nu\uparrow}^0 - v_{\lambda\nu}^*(\vec{r}_i) \gamma_{\nu\downarrow}^0 \right],$$

$$c_{i\lambda\downarrow} = \sum_{\nu} \left[ u_{\lambda\nu}(\vec{r}_i) \gamma_{\nu\downarrow}^0 + v_{\lambda\nu}^*(\vec{r}_i) \gamma_{\nu\uparrow}^0 \right],$$
leading to the Bogolubov- de Gennes (BdG) equations for the amplitudes \( u_{\lambda\nu}(\vec{r}_i) \), \( v_{\lambda\nu}(\vec{r}_i) \) and the eigenenergies \( E_\nu \)

\[
\sum_{\lambda'} \left[ \sum_j K_{ij}^{\lambda\lambda'} u_{\lambda'\nu}(\vec{r}_j) + \Delta(\vec{r}_i) v_{\lambda'\nu}(\vec{r}_i)(1 - \delta_{\lambda\lambda'}) \right] = E_\nu u_{\lambda\nu}(\vec{r}_i), \\
\sum_{\lambda'} \left[ -\sum_j K_{ij}^{\lambda\lambda'} v_{\lambda'\nu}(\vec{r}_j) + \Delta^*(\vec{r}_i) u_{\lambda'\nu}(\vec{r}_i)(1 - \delta_{\lambda\lambda'}) \right] = E_\nu v_{\lambda\nu}(\vec{r}_i),
\]

where the operator \( K_{ij}^{\lambda\lambda'} \) reads

\[
K_{ij}^{\lambda\lambda'} = (\varepsilon_{\lambda'} - \mu) \delta_{ij} \delta_{\lambda\lambda'} + V_{isp}(\vec{r}_i) \delta_{ij} - t_{ij}^{\lambda\lambda'}. \tag{9}
\]

The pairing parameters \( \Delta(\vec{r}_i) \) are, in turn, expressed in terms of the eigenfunctions \( u_{\lambda\nu}(\vec{r}_i) \), \( v_{\lambda\nu}(\vec{r}_i) \) and eigenenergies \( E_\nu \) as [16]

\[
\Delta(\vec{r}_i) = U \sum_\nu (u_{1\nu}(\vec{r}_i)v_{2\nu}^*(\vec{r}_i) + u_{2\nu}(\vec{r}_i)v_{1\nu}^*(\vec{r}_i))(1 - 2f_\nu). \tag{10}
\]

The mean number of particles is given by \( n = \sum_\nu n_\lambda(\vec{r}_i)/L \), where \( L \) is a number of sites in the cluster and

\[
n_\lambda(\vec{r}_i) = \sum_\nu \left[ |u_{\lambda\nu}(\vec{r}_i)|^2 f_\nu + |v_{\lambda\nu}(\vec{r}_i)|^2 (1 - f_\nu) \right]. \tag{11}
\]

In the above formulae \( f_\nu = \left( e^{E_\nu/k_B T} + 1 \right)^{-1} \) denotes the Fermi-Dirac distribution function of quasi-particles.

The local density of states (LDOS) \( N(\vec{r}_i, E) \) is directly accessible in scanning tunneling microscope (STM) measurements and is proportional to the local conductance \( dI(\vec{r}_i, V)/dV \).

In the two - orbital system it is a sum over orbitals of the local densities of states \( N(\lambda, \vec{r}_i, E) \) projected onto respective orbitals

\[
N(\lambda, \vec{r}_i, E) = \sum_\nu |u_{\lambda\nu}(\vec{r}_i)|^2 \delta(E - E_\nu) + |v_{\lambda\nu}(\vec{r}_i)|^2 \delta(E + E_\nu). \tag{12}
\]

Obviously, we have in each site \( N(\vec{r}_i, E) = N(1, \vec{r}_i, E) + N(2, \vec{r}_i, E) \). For a clean system equations (7,8) can be Fourier transformed and written in reciprocal space. For the impure systems with broken translational symmetry, the Bogolubov - de Gennes equations (7 - 10) are solved self-consistently in the real space for a small \( n \times m \) cluster with periodic boundary conditions.

### 3. Clean system

For numerical calculation we include only hopping elements to the nearest-neighbor sites on a square lattice and no hybridization term \( t_{ij}^{\lambda\lambda'} = \delta_{\lambda\lambda'} \delta_{ij}\delta(\delta = \pm x, \pm y) \). The resulting two bands are described by energies \( \varepsilon_\lambda(k_x, k_y) = \varepsilon_\lambda - 2t_\lambda(\cos(k_x) + \cos(k_y)) - \mu \), and we use the following set of parameters: \( t_1 = t \), \( t_2 = 2t \) and \( e_2 - e_1 = 2t \), the interaction strength \( U = 2.5t \) and the number of particles in the system \( n = 1.2 \). \( t \) is our energy unit. With these parameters the bands cross each other along \( \Gamma - X \) and \( \Gamma - M \) lines of the square lattice Brillouin zone for \( \mu = -2t \). It means that for that value of the chemical potential both bands have the same value of the Fermi wave vector \( k_{F1} = k_{F2} \). For the assumed number of electrons in the system \( n = 1.2 \), the narrower band which we denote ‘1’ has larger Fermi wave vector \( k_{F1} > k_{F2} \).
We consider here only the pairs with zero center of mass momentum. The gap parameter in this case is \( \Delta = U \sum_k \langle c_{1,k,\uparrow} c_{2,-k,\downarrow}^\dagger + c_{2,k,\uparrow} c_{1,-k,\downarrow}^\dagger \rangle \) and due to the local character of pairing interaction it includes all the \( \vec{k} \) states in the Brillouin zone. The dependence of \( \Delta \) on the inter-orbital interaction \( U \) for fixed values of the chemical potential \( \mu \) is shown in the figure 1. Note the existence of the critical value of pairing attraction \( U_C(\mu) \) for all positions of the chemical potential except the case where two bands cross each other at the Fermi energy and the system effectively behaves as a typical BCS one. For bands crossing at the Fermi level (homothetic bands) the pairing take place for arbitrarily small attractive interaction. Below \( U_C \) the normal metal has lower free energy than the superconductor.

In a clean two-orbital system one defines partial (projected onto respective orbitals) and total densities of states. They are shown in the figure 2. The partial densities of states are not centered at the chemical potential \( \mu = 0 \). Their sum is centered at the chemical potential and features a number of peaks of different height at positive and negative energies, which are coherence peaks observed in partial densities of states. To understand this let us note, that the eigenvalues of the Bogoliubov-de Gennes equations have the form \( E_\nu = \pm \frac{\varepsilon_1 - \varepsilon_2}{2} \pm \sqrt{(\varepsilon_1 + \varepsilon_2)^2 + \Delta^2} \), where we have suppressed the \( \vec{k} \) dependence of \( \varepsilon_1/2 \). It follows that the gaps in the partial densities of states are centered at the energies \( (\varepsilon_1(k_{F1}) - \varepsilon_2(k_{F1}))/2 \) and \( (\varepsilon_1(k_{F2}) - \varepsilon_2(k_{F2}))/2 \) instead at the Fermi level.

4. Impure system
To study the properties of disordered systems we consider a cluster of 23x17 sites on a square lattice with unit lattice constant with 15% inter-orbital impurities introduced in random sites. Impurities are extended \( V_{\text{imp}}(\vec{r}_i) = V_{12} f_{id} \) with \( f_{id} \) being a number from the Gaussian distribution at sites distance \( id = 0, 1, \sqrt{2}, 2 \) from the impurity center. Other parameters have been assumed to take the same values as in clean superconductor. For a given distribution of impurities, which is shown in the figure 3, and their strength \( V_{12} \) we have solved Bogoliubov-de Gennes equations and calculated local values of the order parameter and density of states. The typical map of the order parameter \( \Delta(\vec{r}) \) in the impure system normalized to its clean system value \( \Delta_0 \) is shown in the figure 4. Comparison of both maps clearly shows that inter-orbital impurities locally suppress the order parameter.
Figure 3. Distribution of the impurity potential $V_{\text{imp}}^{12}(\vec{r})/V^{12}$ in the system of $23 \times 17$ sites. Symbols (+) indicate impurity sites.

Figure 4. The gap maps $\Delta(\vec{r})/\Delta_0$ for the system with inter-orbital impurities $V^{12} = 4t$ and inter-orbital interaction $U = 2.5t$.

More detailed information can be obtained from the local density of states. In the actual calculations of this function we have replaced the Dirac distribution entering formula (12) by the Lorentzian of width $\gamma = 0.05t$. The local densities of states $N(\vec{r}, E)$ for all sites along the line $y = 0$ are shown in the figure 5. The red curves show the density of states at the sites where the impurities are centered. Note the smaller gap values and less distinctive coherence features at the impurity sites. This is in contrast to the typical BCS superconductors for which the coherence peaks are sharper in the impurity sites [17]. The local values of the gap fluctuate from site to site and are visibly smaller in impurity sites.

Figure 5. The local densities of states $N(\vec{r}, E)$ along the line $y = 0$ for the considered system. Red lines indicate position of the impurity sites.

Figure 6. The dependence of the mean order parameter $\langle \Delta \rangle /\Delta_0$ and the critical temperature $T_c/T_{C0}$ on $V^{12}$.

The dependence of the average value of the order parameter normalized to its value in the system without impurities and the superconducting transition temperature on the strength of impurity scattering is shown in the figure 6. The slightly different reaction of $\langle \Delta \rangle$ and $T_c$ is related to inhomogeneous structure of the local gaps as visible in the figure 4. $\Delta_0$ and $T_{C0}$ refer to the clean system.
5. Summary and conclusions
We have studied superconducting properties of the system with inter-orbital pairs. Such system differs from classic one band or two band systems. In particular we have found that:

- there exist critical inter-orbital interaction $U_C$ necessary to stabilize the superconducting state. The value of $U_C$ strongly depends on relative position of both bands and increases with minimal distance between bands at the Fermi level.
- Inter-orbital impurities $V_{12}$ act as a local hybridization. They rather weakly suppress a superconducting order parameter $\Delta$ with respect to the clean case.
- The local density of states is characterized by suppressed coherence features at the impurity sites.

As both, the local density of states $N(\mathbf{r},E)$ and the gap values $\Delta(\mathbf{r})$ can be measured with help of scanning tunneling microscope, the results of this work are subject to experimental verification provided there exist systems in which the present scenario is realized. More detailed analysis of the model in the context of superconducting iron pnictides will be presented elsewhere.

Acknowledgments
This work has been partially supported by the Polish Ministry of Science and Education under the grant No. N N202 2631 38.

References
[1] Bednorz J G and Müller K A 1986 Z. Phys. B 64 189
Müller K A and Bednorz J G 1987 Science 237 1133
[2] Maeno Y, Hashimoto H, Yoshioka K, Nishizaki S, Fujita T, Bednorz J G and Lichtenberg F 1994 Nature 372 532
[3] Nagamatsu J, Nakagawa N, Muranaka T, Zenitani Y and Akimitsu J 2001 Nature 410 63
[4] Kamiyama Y, Hiramatsu H, Hirano M, Kawamura R, Yanagi H, Kamiya T and Hosono H 2006 J. Am. Chem. Soc. 128 10012
Kamiyama Y, Watanabe T, Hirano M and Hosono H 2008 J. Am. Chem. Soc. 130 3296
[5] Suhl H, Matthias B T and Walker L R 1959 Phys. Rev. Lett. 3 552
Moskalenko V A 1959 Fiz. Met. Metallurgiya. 8 503
[6] Sulfrynski M 1962 Phys. Rev. 128 1538
Kondo J 1963 Prog. Theor. Phys. 29 1
Leggett A J 1966 Prog. Theor. Phys. 36 901
[7] Golubov A A and Mazin I I 1997 Phys. Rev. B 55 15146
Bang Y and Choi H Y 2008 Phys. Rev. B 78 134523
Seo K, Bernevig B A and Hu J 2008 Phys. Rev. Lett. 101 206404
Mazin I I and Schmalian J 2009 Physica C: Superconductivity 469 9
[8] Cvetkovic V and Tesanovic Z 2009 Europhysics Lett. 85, 37002.
[9] Dolgov O V, Mazin I I, Parker D and Golubov A A 2009 Phys. Rev. B 79 060502(R)
[10] Kumar N and Sinha K P 1968 Phys. Rev. 174 482
[11] Tahir-Kheli J 1998 Phys. Rev. B 58 12307
[12] Liu W V and Wilczek F 2003 Phys. Rev. Lett. 90 047002
Forbes M M, Gubankova E, Liu W V and Wilczek F 2005 Phys. Rev. Lett. 94 017001
Gubankova E, Mischchenko E and Wilczek F 2006 Phys. Rev. B 74 184516
[13] Moreo A, Daghofer M, Nicholson A and Dagotto E 2009 Phys. Rev. B 80 104507
Gao Y, Su W-P and Zhu J-X 2010 Phys. Rev. B 81 104504
[14] Neto F D, Continentino M A and Lacroix C 2010 J. Phys.: Condens. Matter 22 075701
[15] Bogoliubov N N, Tolmachev V V and Shirkov D V 1958 Fortschr. Phys. 6 605
Valatin G J 1958 Nuovo Cimento 7 843
[16] Ketterson J B and Song S N 1999 Superconductivity (Cambridge: Cambridge University Press)
[17] Ciechan A, Krzyszczak K and Wysokiński K 2009 Journal of Physics: Conference Series 150 052283
Ciechan A and Wysokiński K I 2009 Phys. Rev. B 80 224523