Interorbital pair scattering in clean and impure superconductors

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The calculations of the local and global properties of two band superconductors have been presented with particular attention to the role of the inter-orbital scattering of pairs. The properties of such superconductors are very different from a single band or typical two band systems with dominant intra-band pairing interactions. The role of Van Hove singularity in one of the bands on the properties of intra-band clean superconductor has been discussed. It leads to marked increase of superconducting transition temperature in the weak coupling limit. We study the inhomogeneous systems in which the characteristics change from place to place by solving the Bogolubov-de Gennes equations for small clusters. The suppression of the superconducting order parameter by the single impurity scattering the fermions between bands is contrasted with that due to intra-band impurity scattering. The results obtained for impure systems have been shown as a maps of local density of states, the order parameter and gap function. They can be directly compared with STM spectra of the real material.

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I. INTRODUCTION

Already in the fifties and sixties the main properties of the two band superconductors have been clarified. At that time, however, the existing materials did not show clear evidence of two band behavior. The experimental situation has changed with the discovery of the high temperature superconducting oxides and more with recent discoveries of strontium ruthenate, magnesium diboride and iron pnictides. Even though all of these systems have a number of bands in the vicinity of the Fermi energy their presence shows up in quite a different way.

Magnesium diboride clearly shows two different gaps of the same symmetry. In strontium ruthenate the three band model seems to be necessary to explain its puzzling properties. The model of superconductivity in the iron pnictides is a matter of ongoing debate. The iron pnictides possess a large number of bands around the Fermi energy and few of them seem to play important role in the superconducting state. Two band model has been proposed as minimal model of these superconductors.

With two bands near the Fermi energy one generally expects formation of intra-band and inter-band pairs. In the later case the pairs have in general non-zero center of mass momentum. The simpler case of superconductivity with intraband pairs, which can be scattered between two bands seem to be relevant in modelling of pnictides. Indeed, there are strong theoretical arguments that inter-band interactions may be important in this system. These findings make pnictides different from MgB$_2$, in which main coupling mechanism is intraband. Thus the detailed study of inter-orbital pair scattering mechanism of superconductivity is timely and of importance. The issue has recently been discussed in connection with both cuprate and pnictide superconductors.

In this paper we are mainly interested in the properties of inter-orbital only mechanism of superconductivity. We shall study both clean homogeneous and impure models. Without loss of generality we shall denote two orbitals as 1 and 2. The interaction $U_{11}$ ($U_{22}$) is responsible for superconducting instability inside a band formed by orbitals 1 (2), while $U_{12}$ promotes the scattering of superconducting pair between orbitals 1 and 2. The impurity scattering potential is assumed in general form $\lambda' \gamma' c_{i'\lambda'} c_{i\lambda}$. It scatters electrons from site $i$, orbital $\lambda'$ into orbital $\lambda$ of the same site. If $\lambda = \lambda'$ we call such impurities intra-band, if $\lambda \neq \lambda'$ inter-band.

The organisation of the rest of the paper is as follows. Section 2 presents the general Hamiltonian of the two orbital model and the Bogolubov - de Gennes (BdG) approach used to solve it. The homogeneous superconductors are discussed in Section 3, where we study inter alia the effect of Van Hove singularity in the density of states in one of the bands on the properties of the superconductors with inter-band pair scattering only. The changes induced in the superconductor by single intra-band or inter-band impurity are discussed in Section 4, while the finite concentration of impurities is considered in Section 5. We end up with the discussion of our results and their relevance to most prominent two band superconductors: MgB$_2$ and iron pnictides.

II. HAMILTONIAN FOR THE TWO ORBITAL SUPERCONDUCTOR

We start with general Hamiltonian in a real space describing the system with two orbitals. We assume the spin-independent effective pairing interaction between fermions in various orbital states. The randomness in the system is easily incorporated via site dependence of...
parameters. The Hamiltonian reads
\[ H = \sum_{ij,j',\lambda',\sigma} \left( -t_{ij}^{\lambda\lambda'} + V_{\text{imp}}^{\lambda\lambda'}(\vec{r}_i) \delta_{ij} \right) c_{ij\lambda\sigma}^+ c_{ij'\lambda'\sigma} + \sum_{i,\lambda,\sigma} (\epsilon_\lambda - \mu) c_{i\lambda\sigma}^+ c_{i\lambda\sigma} + \sum_{i,\lambda_1,\lambda_2,\lambda_3,\lambda_4} U_{\lambda_1,\lambda_2,\lambda_3,\lambda_4}(\vec{r}_i) c_{i\lambda_1\lambda_2}^+ c_{i\lambda_3\lambda_4}^+ c_{i\lambda_4\lambda_1} c_{i\lambda_2\lambda_3}, \] (1)
where \( c_{ij\lambda\sigma}^+ \) and \( c_{i\lambda\sigma}^+ \) are creation and annihilation operators of electrons with spin \( \sigma = \uparrow, \downarrow \) at the lattice site \( \vec{r}_i = i \) in the orbital \( \lambda \). \( \epsilon_\lambda \) is the electron energy and \( \mu \) is the chemical potential. \( t_{ij}^{\lambda\lambda'} \) is the hopping integrals between the same or different orbitals (if \( \lambda \neq \lambda' \)). \( U_{\lambda_1,\lambda_2,\lambda_3,\lambda_4}(\vec{r}_i) \) denotes interactions, which are attractive for \( U_{\lambda_1,\lambda_2,\lambda_3,\lambda_4}(\vec{r}_i) < 0 \). The dependence of the interaction parameters on the position \( \vec{r}_i \) allows to treat systems with inhomogeneous pairing.

We use standard mean-field decoupling valid for a spin singlet superconductor and get the following effective Hamiltonian
\[ H^{\text{MFA}} = \sum_{ij,j',\lambda,\lambda',\sigma} \left( -t_{ij}^{\lambda\lambda'} + V_{\text{imp}}^{\lambda\lambda'}(\vec{r}_i) \delta_{ij} \right) c_{ij\lambda\sigma}^+ c_{ij'\lambda'\sigma} + \sum_{i,\lambda,\sigma} (\epsilon_\lambda + V_{\lambda,\sigma}(\vec{r}_i) - \mu) c_{i\lambda\sigma}^+ c_{i\lambda\sigma} + \sum_{i,\lambda,\lambda'} \left( \Delta_{\lambda\lambda'}(\vec{r}_i) c_{i\lambda\lambda'}^+ c_{i\lambda'\lambda} + \text{h.c.} \right), \] (2)
where the order parameters \( \Delta_{\lambda\lambda'}(\vec{r}_i) \) are related to the pairing correlation functions \( f_{\lambda\lambda'}(\vec{r}_i) = \langle c_{i\lambda\uparrow}^+ c_{i\lambda'\downarrow} \rangle \) through
\[ \Delta_{\lambda_1,\lambda_2}(\vec{r}_i) = -\sum_{\lambda_3,\lambda_4} U_{\lambda_1,\lambda_2,\lambda_3,\lambda_4}(\vec{r}_i) f_{\lambda_3\lambda_4}(\vec{r}_i). \] (3)
The local Hartree terms \( V_{\lambda}(\vec{r}_i) \) depend on the number of particles at given site \( n_{\lambda\sigma}(\vec{r}_i) = \langle c_{i\lambda\sigma}^+ c_{i\lambda\sigma} \rangle \).
\[ V_{\lambda}(\vec{r}_i) = \sum_{\lambda'} U_{\lambda,\lambda',\lambda}(\vec{r}_i) n_{\lambda',\lambda}(\vec{r}_i). \] (4)
We consider here only diagonal correlations \( \langle c_{i\lambda\sigma}^+ c_{i\lambda'\sigma'} \rangle = \delta_{\lambda\lambda'} \delta_{\sigma\sigma'} n_{\lambda\sigma}(\vec{r}_i) \).

The Hamiltonian \([\text{2}]\) is diagonalised with help of the Bogolubov - Valatin transformation\([\text{29-30}]\)
\[ c_{i\lambda\lambda'} = \sum_{\nu} \left( u_{\lambda\nu}(\vec{r}_i) \gamma_{\nu\downarrow}^\dagger - v_{\lambda'\nu}(\vec{r}_i) \gamma_{\nu\uparrow}^\dagger \right), \] (5)
\[ c_{i\lambda\lambda'} = \sum_{\nu} \left( u_{\lambda\nu}(\vec{r}_i) \gamma_{\nu\uparrow} + v_{\lambda'\nu}^*(\vec{r}_i) \gamma_{\nu\downarrow}^\dagger \right) \] (6)
leading to the Bogolubov- de Gennes (BdG) equations for amplitudes \( u_{\lambda\nu}(\vec{r}_i), v_{\lambda'\nu}(\vec{r}_i) \) and eigenenergies \( E_\nu \)
\[ \sum_{j,\lambda'} K_{ij}^{\lambda\lambda'} u_{\lambda'\nu}(r_j) + \sum_{\lambda'} \Delta_{\lambda\lambda'}(\vec{r}_i) v_{\lambda'\nu}(\vec{r}_i) = E_\nu u_{\lambda\nu}(\vec{r}_i), \] (7)
\[ -\sum_{j,\lambda'} K_{ij}^{\lambda\lambda'} v_{\lambda'\nu}(r_j) + \sum_{\lambda'} \Delta_{\lambda\lambda'}(\vec{r}_i) u_{\lambda'\nu}(\vec{r}_i) = E_\nu v_{\lambda\nu}(\vec{r}_i), \] (8)
where the operator \( K_{ij}^{\lambda\lambda'} \) reads
\[ K_{ij}^{\lambda\lambda'} = (\epsilon_\lambda - \mu + V_{\lambda\sigma}(\vec{r}_i)) \delta_{ij} \delta_{\lambda\lambda'} + V_{\text{imp}}^{\lambda\lambda'}(\vec{r}_i) \delta_{ij} - t_{ij}^{\lambda\lambda'}. \] (9)
The pairing parameters \( \Delta_{\lambda\lambda'}(\vec{r}_i) \) and Hartree potentials \( V_{\lambda}(\vec{r}_i) \) are in turn expressed in terms of eigenfunctions and eigenenergies \( u_{\lambda\nu}(\vec{r}_i), v_{\lambda\nu}(\vec{r}_i), E_\nu \) as\([\text{2}]\)
\[ n_{\lambda}(\vec{r}_i) = \sum_{\nu} \left( |u_{\lambda\nu}(\vec{r}_i)|^2 f_\nu + |v_{\lambda\nu}(\vec{r}_i)|^2 (1 - f_\nu) \right), \] (10)
\[ f_{\lambda\lambda'}(\vec{r}_i) = \sum_{\nu} \left[ u_{\lambda\nu}(\vec{r}_i)v_{\lambda'\nu}^*(\vec{r}_i)(1 - f_\nu) - u_{\lambda'\nu}(\vec{r}_i)v_{\lambda\nu}^*(\vec{r}_i)f_\nu \right]. \] (11)
In the above formulae \( f_\nu = (e^{E_\nu/k_B T} + 1)^{-1} \) denotes the Fermi-Dirac distribution function of quasi-particles. The total number of particle in the given band (to be denoted by the same index as the orbital) is given by \( N_\lambda = \sum_{\nu} n_{\lambda\nu}(\vec{r}_i) \).

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 band system it is a sum of local densities of states of the individual bands \( N(\lambda, \vec{r}_i, E) \)
\[ N(\lambda, \vec{r}_i, E) = \sum_{\nu} |u_{\lambda\nu}(\vec{r}_i)|^2 \delta(E - E_\nu) + |v_{\lambda\nu}(\vec{r}_i)|^2 \delta(E - E_\nu). \] (12)
Obviously we have at each site \( N(\vec{r}_i, E) = N(1, \vec{r}_i, E) + N(2, \vec{r}_i, E) \). For a clean system equations \([\text{7,8}]\) can be Fourier transformed and written (in closely analogous form) in reciprocal space. For the impure systems with broken translational symmetry the Bogolubov - de Gennes equations \([\text{7,8}]\) are solve self-consistently in real space for a small \( n \times n \) cluster with periodic boundary conditions. For a two orbital model the typical size of the cluster is \( 20 \times 30 \). In the next section we start with the comparison of our real space (for small cluster) calculations with (numerically) exact results obtained in reciprocal space (i.e. for bulk system).

III. HOMOGENEOUS SUPERCONDUCTORS

In this section we shall discuss some properties of homogeneous two band superconductors paying special attention to the comparison of the accuracy of small cluster calculations with bulk system. We also consider the effect of Van Hove singularity in one of the bands on the properties of inter-band pairing superconductivity and the role of various inter-band couplings.

A. Small clusters vs. bulk systems

We start with the homogeneous system with two orbitals denoted 1 and 2. The superconductor is de-
scribed by the following set of parameters. The interband interaction has the form of pair scattering only \( U_{12} = U_{1122} \), while two intra-band interactions are \( U_{11} = U_{1111} \) and \( U_{22} = U_{2222} \). We consider two-dimensional square lattice with non-zero hopping integrals between the nearest neighbor sites only \( t_\lambda = t_{ij}^\lambda \) and hybridization \( t_{ij} = t_{ij}^{12} \). We set the direct hoping between orbitals no. 1 as our energy unit \( t_1 = t = 1 \). Since we are ignoring the possibility of inter-orbital pairs, we use the simpler notation \( \Delta_1 = \Delta_{11} \) and \( \Delta_2 = \Delta_{22} \).

Fig. 1 shows the single particle energy bands along main symmetry direction in the two dimensional Brillouin zone obtained for the following set of parameters \( e_2 - e_1 = 2t, t_1 = t, t_2 = 2t, t_{12} = 0.05t \). The chemical potential \( \mu = 0 \) and the total number of carriers \( n = 1.62 \).

Fig. 2 compares the solutions obtained for the bulk system with those for small clusters of various size. We consider here the bulk data as exact. The accuracy of determination of the gap parameter for bulk homogeneous system (in our case assumed to be of the order of \( 10^{-4}t \)) is only limited by the time of calculations. We have found that at the band center the results obtained for clusters with size greater than 400 sites are acceptable. Relative changes of the gaps with respect to the bulk values

\[
\delta \Delta_\lambda = (\Delta_\lambda(L) - \Delta_\lambda^{\text{bulk}})/\Delta_\lambda^{\text{bulk}} \cdot 100%
\]

are in the range of \( \delta \Delta_1 < 0.15\% \) in the first band and slightly greater \( \delta \Delta_2 < 1.5\% \) for the second band. Well inside the bands the spectrum is quasi-continuous and the results agree very well with bulk data but near the band edges the spectrum of finite clusters is discrete and the differences are larger (c.f. Fig. 2).

**B. Inter-orbital pairing only superconductor - the role of Van Hove singularity**

As a general rule one finds that the inter-orbital scattering \( U_{12} \) plays a minor role in superconductors with dominant intra-band interactions. This interaction, however, couples two bands and may lead to the increase of the superconducting transition temperature. The situation changes drastically if the inter-band pairing is the only existing interaction. The properties of the superconductors with dominant inter-band scattering are markedly different from those with dominant intra-band interactions. In particular, the superconducting transition takes place for arbitrary sign of \( U_{12} \). The value of the gap in the first band is determined by the interaction \( U_{12} \) and the density of states in the second band and vice versa, the gap in the second band is proportional to the partial density of states (DOS) at the Fermi level in the first band. This can easily be seen from the general two band BCS equations

\[
\Delta_1(1 + U_{11} F_1) = -U_{12} \Delta_2 F_2,
\]

\[
\Delta_2(1 + U_{22} F_2) = -U_{12} \Delta_1 F_1,
\]

where

\[
F_\lambda = \int_0^{\hbar \omega_c} dE N_\lambda(E) \frac{\tanh \frac{\sqrt{E^2 + \Delta_\lambda^2}}{2k_B T}}{\sqrt{E^2 + \Delta_\lambda^2}}
\]

and \( N_\lambda(E) \) denotes single particle density of states in the band \( \lambda \). In this discussion we interested in the limit of inter-band pair scattering only. For \( U_{11} = U_{22} = 0 \) the above equations reduce to

\[
\Delta_1 = -U_{12} \Delta_2 \int_0^{\hbar \omega_c} dE N_\lambda(E) \frac{\tanh \frac{\sqrt{E^2 + \Delta_\lambda^2}}{2k_B T}}{\sqrt{E^2 + \Delta_\lambda^2}}.
\]
\[ \Delta_2 = -U_{12}\Delta_1 \int_0^{\hbar \omega_c} dE N_1(E) \frac{\tanh \sqrt{E^2 + \Delta_1^2} / 2k_B T}{\sqrt{E^2 + \Delta_1^2}}. \]  

(15)

It is clear from equations (15) that the value of \( \Delta \) in the second band is determined by the density of states in the first one and vice versa. It is also obvious that the nonzero solutions can be obtained for both signs and arbitrary small value of the coupling \( U_{12} \). For positive value of \( U \) the order parameters in the two bands have opposite signs, while for negative \( U_{12} \) they are of the same sign. The inter-orbital pairing model has a number of unusual features. It has been found\textsuperscript{28,35} that the ratio \( \Delta_2 / \Delta_1 = \sqrt{N_1 / N_2} \), where \( N_2(N_1) \) is the density of states in band 2(1) at the Fermi level and the superconducting transition temperature of the system is given by the BCS-like expression

\[ T_c = 1.136 \frac{\hbar \omega_c}{k_B} \exp \left( -\frac{1}{\lambda_{eff}} \right) \]  

(16)

with \( \lambda_{eff} = \lambda_0 = \sqrt{U_{12}^2 N_1 N_2} \).

It often happens that the Fermi level in superconductors lies close to the Van Hove singularity. In layered systems with nesting properties of the (quasi - two dimensional) Fermi surface the density of states near the Van Hove singularity changes logarithmically

\[ N(E) = N_0 \ln(2W/|E|) \Theta(|E| - W) \]  

(17)

with \( W \) being the band width and \( \Theta(x) \) the step function. It is known that the existence of such singularity modifies\textsuperscript{36} the BCS expression for the transition temperature (16). In particular, in the one band case and the weak coupling limit\textsuperscript{37} \( \lambda \ll 1 \) it leads to increase of the superconducting transition by changing the effective interaction: \( 1/\lambda_{eff} = \sqrt{2} / \lambda \).

Here we assume the density of states in the second band to be singular \( N(2, E) = N_2 \ln(2W/|E|) \) near the Fermi energy, while that of the first band flat \( N(1, E) = N_1 \). Near \( T_c \) equations (15) are linearised, we approximate \( \tanh(x) \approx \min(x, 1) \) and find (we use here \( \hbar = k_B = 1 \))

\[ \Delta_1 = -\Delta_2 U_{12} N_2[1 + \ln \frac{2W}{\omega_c} + \ln \frac{\omega_c}{2T_c}] + \ln \frac{2W}{\omega_c} \frac{\omega_c}{2T_c} + \frac{1}{2} (\ln \frac{\omega_c}{2T_c})^2 \]

\[ \Delta_2 = -\Delta_1 U_{12} N_1[1 + \ln \frac{\omega_c}{2T_c}] \]  

(18)

The analysis of the above set of equations in the weak coupling limit \( (U_{12} \to 0) \) leads to the approximate BCS like expression for the superconducting transitions temperature with \( \lambda_{eff} = \frac{\Delta_2}{\Delta_1} = \left( \frac{U_{12} N_1 N_2}{N_2} \right)^{1/3} \) and to the modification of the prefactor, which changes from 1.136\( \omega_c \) to 1.136\( \omega_c (2W/\omega_c)^{2/3} \). It is interesting to note that up to the prefactor the Van Hove singularity in one of the bands increases \( T_c \) of intra-band superconductor at the very weak coupling only \( \lambda_0 \ll 1 \).

In a similar way one can calculate the effect of Van Hove singularity on the ratio of the gaps \( \Delta_2 / \Delta_1 \) at zero temperature. One finds

\[ \Delta_1(0) = -\Delta_2(0) U_{12} N_2[1 - \ln \frac{\Delta_2(0)}{2W} - \frac{1}{2} (\ln \frac{\omega_c}{2W})^2 + \frac{1}{2} (\ln \frac{\Delta_2(0)}{2W})^2] \]

\[ \Delta_2(0) = -\Delta_1(0) U_{12} N_1 \ln \frac{2\omega_c}{\Delta_1(0)} \]  

(19)

Even in the extreme weak coupling limit \( \lambda_0 \to 0 \) when \( T_c, \Delta_1, \Delta_2 \to 0 \) the gap ratio is not given by the ratio of the densities of states and depends on \( T_c \) and thus \( \lambda_0 \). The ratio \( \Delta_2 / \Delta_1 \) decreases from the value much larger than \( \sqrt{N_1 / N_2} \) for small \( \lambda_0 \) to values below \( \sqrt{N_1 / N_2} \) for larger \( \lambda_0 \). However, it is interesting to note that the correct description of the intra-band superconductivity requires the strong coupling theory\textsuperscript{38}, even if \( \lambda_0 < 1 \) and Van Hove singularity plays similar role in Eliashberg equations\textsuperscript{39}.

C. The role of the band couplings

Before the presentation of the real space local properties of the model with general interactions we spent here some time on discussing the homogeneous systems and the influence of model parameters on the superconducting bulk state. In particular, we are interested in the dependence of superconducting state on the couplings between bands. The hybridization parameter \( t_{12} \) provides single particle coupling and the inter-band pair scattering \( U_{12} \) provides the direct two body inter-band interaction. The hybridization changes single particle spectrum and this influences the superconductivity.

Fig. 4 (left panel) shows the changes of the order parameter in the first band due to increase of hybridization \( t_{12} \). The strong decrease of \( \Delta_1 \) with \( t_{12} \) results from the changes of the single particle spectrum in the first band. The second band is essentially decoupled, as \( U_{12} = 0 \). One observes strong decrease of the projected density of states around the Fermi level in both bands. This is illustrated in the figure 4. Left panel shows the total (dashed curve) and projected onto orbital 1 and 2 densities of states in the system without any inter-band coupling \( (t_{12} = 0) \), while in the right panel for strong hybridization \( t_{12} = 5t \).

As mentioned, the inter-band interaction alone leads to the superconducting instability independently if it is repulsive or attractive. It induces gaps in both bands. The results are shown in the right panel of Fig. 3. The value of the gap in the second band is larger because the density of states near \( E_F \) in the first band is larger (c.f. equations (15)).

The simultaneous presence of the inter-band \( (U_{12}) \) and intra-band \( (here U_{11} only) \) interactions results in an in-
In this section we study a single short-ranged non-magnetic impurity embedded in an otherwise clean system. We solve BdG equations (7) and (8) on a small cluster of size $L = 13 \times 17$ with an impurity placed in its center. In the two orbital model the impurity may scatter electron from a given orbital to the same orbital (intra-orbital scattering to be denoted $V_{imp}^{1(2)}$) or to other orbital (inter-orbital scattering - $V_{imp}^{12}$) located at the same site. The inter-band scatterers were intensively studied in connection with MgB$_2$. It has been found that Eliashberg theory leads to much slower rate of $T_c$ suppression than predicted on the basis of BCS treatment. Here we allow for both, the intra-band and inter-band pairing interactions and compare the $T_c$ changes induced by two types of impurities. Instead of strong coupling Eliashberg approach we are using Bogolubov-de Gennes approach which allows for the distortion of the wave function around impurity and is more suitable to treat inhomogeneous superconductors than either BCS or Eliashberg (both $k$-space based) theories.

We consider the system described by the following set of parameters $e_2 - e_1 = 2t, t_1 = t, t_{12} = 2t, t_{12} = 0.05$ and $n = 1.2$, and start with the pairing interaction in the first band band only: $U_{11} \neq 0, U_{12} = 0$. Due to the weak hybridization $t_{12} = 0.05t$ there exist small coupling between bands. Figure (6) illustrates the changes in the order parameter $\Delta_1$ around intra-band (left panel) and inter-band (right panel) impurity. Note different patterns of changes in $\Delta_1$. The intra-band impurity more strongly suppresses order parameter at the impurity site and leads to slight increase of it (with respect to the value for homogeneous system) at nearest neighbor sites. The inter-band impurity scattering on the other hand diminishes the order parameter at the impurity site and around it, but slightly less for next-nearest neighbors than for nearest-neighbors. In spite of its short range the inter-band impurity modifies the order parameter at distances larger than intra-band one. For the parameters used the clean system has $\Delta_1 = 1.07t$ At the impurity site one finds $\Delta_1(0,0) = 0.17t$ for $V_{imp}(r_i) = V_{imp}^{12}(r_i)$ and $\Delta_1(0,0) = 0.11t$ for $V_{imp}(r_i) = V_{imp}^{1}(r_i)$.

In figure (7) we show the local quasiparticle density of states at the impurity site $\vec{r} = (0,0)$ and its nearest $(0,1)$ and next-nearest $(1,1)$ neighbor sites. The inter-band impurity induces states inside the gap.

The interesting aspect of these studies is connected with the fact that the effect of $V_{imp}^{12}$ depends on the sign of inter-band interaction $U_{12}$. There is no similar dependence connected with intra-band impurities ($V_{imp}^{1}$ or $V_{imp}^{2}$). This is illustrated in the Fig. (8). The changes
for attractive inter-band interaction (note that positive density of states projected onto orbital 1, at the impurity site (0,0) is almost zero).

FIG. 6: The influence of intraband \( V_{imp}^{1}(\vec{r}_i) \) (left panel) and interband \( V_{imp}^{12}(\vec{r}_i) \) (right panel) impurity of the same strength (=4t) on the local values of \( \Delta_1(\vec{r}_i) \) in a superconductor with \( U_{11} = -3.5t, U_{12} = 0 \).

FIG. 7: The energy dependence of the local quasiparticle density of states projected onto orbital 1, at the impurity site (0,0) and its neighbors for system with intraband (left panel) and interband (right panel) impurities for \( U_{11} = -3.5t, U_{12} = 0 \).

of the order parameters in the first and second bands clearly depend on the sign of inter-band interaction. For the clean system we have \( |\Delta_1| = 2.69t, |\Delta_2| = 2.07t \). At the inter-band impurity site we have found \( |\Delta_1| = 1.61t \) and \( |\Delta_2| = 1.21t \) for \( U_{12} = -5t \), i.e. roughly 40% reduction. On the other hand in the superconductor with \( U_{12} = +5t \) we find at the impurity site \( |\Delta_1| = 0.20t \) and \( |\Delta_2| = 0.23t \). The order parameters are suppressed only few times stronger in the superconductor with repulsive inter-orbital interaction.

Similar effect has earlier been noted within the weak coupling Eliashberg theory for finite (inter-orbital) impurity concentration in the two band superconductors. Here we observe similar behavior already for the single impurity. The feature is further discussed in the next section for a system with finite concentration of impurities. Performing analytical studies of the \( T_c \) suppression in two band case the authors have noted that strong suppression of superconductivity for finite concentration of inter-band impurities is to be expected for the inter-band couplings fulfilling the inequality

\[
U_{12} \geq -\frac{N_1^2U_{11} + N_2^2U_{22}}{2N_1N_2}.
\] (20)

It other words much weaker suppression of \( T_c \) is expected for attractive inter-band interaction (note that positive interactions are attractive in the notation of the paper).

FIG. 8: The changes of the order parameters around inter-band impurity \( V_{imp}^{12}(\vec{r}_i) \) located at the center of the superconducting cluster with \( U_{11} = -3.5t \). Left panels are for \( U_{12} = -5t \), middle panels for \( U_{12} = 5t \). The right panels show the maps of difference between values of the order parameter for attractive and repulsive interband interaction.

FIG. 9: The energy dependence of the quasiparticle density of states at the interband impurity \( V_{imp}^{12}(\vec{r}_i) \) and the neighboring sites for attractive (left panel) and repulsive (right panel) interband pairing interaction.

In more detail this is again illustrated in Fig. 9, which shows the energy dependence of the quasiparticle density of states at and near the impurity site for attractive (left panel) and repulsive (right panel) inter-band interaction. In the later case the order parameter at the impurity site and around it is strongly suppressed and new states appear inside the gap. The intra-band impurity scattering (not shown) is not effective in suppressing superconductivity independently of the \( U_{12} \) sign. This is due to the same mechanism (Anderson theorem) as for single band s-wave superconductors.

It is also of interest to look at the relative phases of the order parameters near the impurity in the superconductor with \( U_{12} > 0 \). As noted earlier for repulsive inter-orbital interactions the \( s_\pm \)-wave pairing state is realised. This state has s-wave like order parameters on two Fermi surfaces, the phases of which differ by \( \pi \). It means that if the phase of \( \Delta_\lambda \) on one of the Fermi surfaces is \( \phi \), the phase on the other is \( \phi + \pi \). This phase relation is in fact responsible for strong suppression of superconductivity by inter-band impurities. It turns out that at the \( V_{imp}^{12} \) impurity site the phases of the gaps change by \( \pi \) with respect to the phases in the bulk. Obviously, there
is no such effect for attractive inter-band interaction.

V. MANY IMPURITIES IN THE TWO BAND SUPERCONDUCTOR

In this section we consider the two band impure superconductor with inter-band and intra-band impurities. Our sample has a rectangular shape. It is \( L = 17 \times 21 \) sites large with a square lattice of unit lattice constant. It contains 20\% inter-band or intra-band impurities randomly distributed. We are not averaging over distribution of impurities, but rather calculate the local property at each site and present the result in the form of maps.

To make the impurities more realistic we assume that they are extended \( V_{\text{imp}}(\vec{r}) = V_{\lambda\lambda} f_{\text{id}} \) with \( f_{\text{id}} \) being a number from the Gaussian distribution at sites distance \( id = 1, \sqrt{2}, 2 \) from the impurity. The superconductor studied in this Section is characterized by one active band with \( U_{11} = -3.5t \) and inter-band interaction \( |U_{12}| = 5t \). The other parameters are: \( e_2 - e_1 = 2t, t_1 = t, t_2 = 2t, t_{12} = 0.05 \) and \( \eta = 1.2 \). Energies are measured in units of \( t \) with respect to chemical potential.

Figures (10) and (11) show the suppression of the order parameters in the two bands for intra-band and inter-band impurities, respectively. In all cases one observes similar patterns and large degree of (anti)correlation between the impurity positions and the gap values. However, the inter-band impurities suppress order parameters in both bands much less for \( U_{12} = -5t \) than for opposite sign of this coupling. For negative \( U_{12} \) the phases of the order parameters on two Fermi surfaces are the same and the scattering of a pair from band 1 into band 2 is harmless, as the superconductor as a whole looks like s-wave one, and is protected against impurities by the Anderson theorem.\(^\text{10}\)

Even though the maps presenting suppression of the order parameters by the intra-band and inter-band impurities shown in the Figures (10) and (11) look to large extend similar the big differences are observed in the local densities of states. They are shown in figures (12) and (13). Left panels of both figures show the local densities of states as function of energy along the line \( x = -7 \) in the first band. Middle panels present the results for the second band and the total DOS is plotted in right panels along the same cut. Intra-band impurities, Fig. (12) induce large inhomogeneities, which show up as gaps in the local density of states of amplitude strongly changing from site to site. Sites close in space may have largely different gaps. Similarly, the inter-band impurities in a superconductor with large attractive inter-band scattering also induce inhomogeneities. However, they are much smaller (recall for the same distribution and strength of impurities). The gaps also change from site to site, but more gradually i.e. on larger spatial scale. On the contrary, the same inter-band impurities nearly completely destroy the superconductivity in the system with strong repulsive inter-band pair scattering i.e. in the \( s_{\pm} \) state.

Different reaction of the system with repulsive and attractive inter-band interactions to impurities may well be characterized by the dependence of the superconducting transition temperature \( T_c \) or the average gap on the strength of \( V_{\text{imp}} \). In the left panel of the Fig. (14) we show the relative change of \( < \Delta_1 + \Delta_2 > \) in the impure system normalized to its clean value \( < \Delta_1 + \Delta_2 > \) with increasing the strength of intra-band impurities \( V_{\text{imp}} = V_{\text{imp}}^1 = V_{\text{imp}}^2 \) (dashed curve with triangles) and on inter-band impurities \( V_{\text{imp}} = V_{\text{imp}}^{12} \) in a system with \( U_{12} = -5t \) (curve with full squares) or \( U_{12} = +5t \) (curve with dots). The right panel of that figure shows the changes in \( T_c \) with \( V_{\text{imp}}^{12} \) for two signs of inter-band scattering. In a qualitative agreement with the results of
FIG. 12: Partial (left and middle panel) and total (right panel) density of states as a function of energy close to the Fermi energy at the sites along the line $x = -7$ of the same sample as shown in the figure [10].

FIG. 13: The energy dependence of the partial and total densities of states $N(\lambda, y, E)$ at the sites along the line $x = -7$ of the sample shown in figure 11. The upper row corresponds to attractive inter-band interaction, while the lower to repulsive one.

Kogan et al. observe much stronger diminishing of $T_c$ normalized to its clean system value $T_{c0}$ for repulsive than for attractive $U_{12}$. Similar dependence of $T_c$ on impurity strength for both signs of $U_{12}$ at small disorder is attributed to our use of Bogoliubov - de Gennes approach which is more suitable to study inhomogeneous systems than the Eilenberger or BCS theories. In BdG approach the condensate wave function may distort around the impurity and this allows the system to keep its condensation energy and $T_c$ much higher than it would result from Abrikosov-Gorkov approach to impure superconductors, which does not allow for a local changes in the wave function.

VI. DISCUSSION AND CONCLUSIONS

We have studied the model of two band superconductor with intra-band and inter-band interactions. In the present paper we concentrated on some general aspects of the two band model. In particular we have found that the presence of Van Hove singularity in the density of states in one of the bands leads to strong enhancement of the superconducting transition temperature of intra-band only superconductor in the weak coupling, i.e. for $\lambda_0 \ll 1$. However, neglecting changes of prefactor, the mere increase of effective interband coupling by Van Hove singularity seem to be not large enough to make the electron-phonon coupling responsible for superconductivity, at least so in LaFeAsO for which the coupling constant matrix has been found with $\lambda_{12} = 0.093$ and $\lambda_{21} = 0.124$. Interestingly, our analysis suggests that for elevated values of $\lambda_0$ the effect of Van Hove singularity is to diminish $T_c$ in comparison to the system without logarithmic enhancement of DOS. The model with both types of pairing interactions leading to $s -$ or $s_{\pm}$-wave symmetry displays number of features similar to that observed in real many band materials, particularly MgB$_2$ and iron pnictides.

MgB$_2$ is a well established superconductor with two gaps. It is believed to have one active band and relatively weak inter-band coupling. Its much slower than predicted by the Abrikosov-Gorkov theory suppression of the superconducting transition temperature by impurities may point towards the inter-band character of impurities and repulsive character of inter-band pair scattering ($U_{12} > 0$). Such a case is illustrated in the upper row of Fig. 13.

Another prominent recent example of the many band superconductors is provided by the iron pnictides. These superconductors seem to belong to different class of many band materials in which the inter-band interaction is dominant and the order parameter has different signs on different Fermi surface sheets - the $s_{\pm}$ state. The existing samples are certainly strongly disordered, as it can be inferred from large values of resistance just above $T_c$. Despite large disorder they are superconduct-
ing with quite large $T_c$. This suggests $s$- or $s_\pm$-wave like order parameter. As we have seen the superconductor with dominant attractive $U_{12}$ interactions is quite robust against impurities, both of intra- and (and even more) inter-band type (c.f. figures [12] and [13]).

The robustness of the two band superconductors with attractive inter-band interactions to the impurities can be traced back to the Anderson theorem. On the other hand the $s_\pm$ state induced in two band model by repulsive inter-band interactions is characterized by large sensitivity to inter-band impurity scattering. These results are in agreement with previous studies of similar models [38,39].

The maps plotted in the Figs. [11] and [10] are in qualitative agreement with recent scanning tunnelling microscopy (STM) studies for pnictide superconductors [48,49,50]. In these papers the relatively small variation of the local gaps have been observed with the average gap $\Delta = 6 - 7 \meV$ and $2\Delta(0)/k_B T_c \approx 7$ indicating strong coupling superconductivity. The detailed analysis of the STM spectra in pnictides will be the subject of future studies.

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