Cooper pairs in a two-orbital superconductor: bands filling effect on pair sizes

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Abstract. The two-orbital superconducting state is modeled by on-site intra-orbital negative-$U$ Hubbard correlations together with inter-orbital pair-transfer interactions. The influence of bands filling on the temperature dependencies of the sizes of Cooper pairs in different orbitals is analyzed. It is found that the sizes exhibit unconventionally strong variation in the temperature scale for occupations favouring interband proximity effect.

1. Introduction
Multi-component superconductivity models, developed more than fifty years starting from the papers \cite{1, 2, 3}, have been an object of growing interest. The research activity in this direction has been especially stimulated by the acceptance of the multi-gap superconductivity in MgB$_2$ \cite{4}, cuprates \cite{5} and iron-arsenic compounds \cite{6}.

Due to the interaction between electron pairing amplitudes caused by interband pair-transfer processes the properties of two-band systems may be rather different from the corresponding characteristics in one-band superconductors. In particular, such quantities as coherence lengths cannot be attributed to the definite bands and must be treated as the characteristics of whole two-component condensate \cite{7, 8, 9, 10, 11}. The characteristic lengths of coherency as well as magnetic field penetration depth in a two-orbital superconductor described by the negative-$U$ Hubbard model \cite{12} were examined in \cite{11, 13, 14} as the functions of bands filling and various orbital parameters.

As opposed to coherence lengths which are characteristics of joint condensate, the Cooper pairs remain attached with the certain bands (orbitals).

In what follows we study the behaviour of the sizes of Cooper pairs vs temperature for various bands fillings in the two-orbital negative-$U$ Hubbard model of superconductivity. Note that other limits are also possible. Namely, for iron-based systems, magnesium diboride, and other novel superconducting materials transition to BEC and BCS-BEC crossover scenario have been proposed \cite{15}. Such limits open new possibilities of phenomenon descriptions including the reformulation of the Cooper pairs role in superconductivity \cite{16} but they are associated with stronger coupling which is not considered in the present report.
2. Two-orbital superconductivity

We start with the Hamiltonian of the two-orbital model\cite{11, 17} of the following form:

\[
H = \sum_{i} \sum_{\alpha} \sum_{\sigma} \left[ t_{ij}^{\alpha} \delta_{ij} + (\epsilon_{ij}^{\alpha} - \mu) \right] a_{i\alpha\sigma}^+ a_{j\alpha\sigma} + \frac{1}{2} \sum_{\alpha} \sum_{i} \sum_{\sigma} U_{i\alpha\sigma} n_{i\alpha\sigma} n_{i\alpha-\sigma} + \frac{1}{2} \sum_{\alpha,\alpha'} \sum_{i} \sum_{\sigma} U_{i\alpha\sigma}^2 a_{i\alpha\sigma}^+ a_{i\alpha'\sigma}^+ a_{i\alpha-\sigma} a_{i\alpha'-\sigma},
\]

where \(a_{i\alpha\sigma}^+ (a_{i\alpha\sigma})\) is the electron creation (destruction) operator in the orbital \(\alpha = 1, 2\) localized at the site \(i\); \(\sigma\) is the spin index; \(t_{ij}^{\alpha}\) is the hopping integral; \(\epsilon_{ij}^{\alpha}\) is the orbital energy; \(\mu\) is the chemical potential; \(U_{i\alpha\sigma} < 0\) is the intra-orbital attraction energy; \(n_{i\alpha\sigma} = a_{i\alpha\sigma}^+ a_{i\alpha\sigma}\) is the particle number operator; \(U_{i\alpha\sigma}^2\) with \(\alpha \neq \alpha'\) is the inter-orbital interaction energy.

In the reciprocal space one obtains in the mean-field approximation the Hartree-Fock-Gorkov self-consistent equations

\[
\sum_{\alpha} n_{\alpha} = N^{-1} \sum_{\alpha} \sum_{k} \sum_{\sigma} \left< a_{ok\sigma}^+ a_{ok\sigma} \right>,
\]

\[
\Delta_{\alpha} = N^{-1} \sum_{\alpha'} \sum_{k} U_{\alpha\alpha'} \left< a_{\alpha'k\uparrow}^+ a_{\alpha'k\downarrow} \right>
\]

with

\[
\left< a_{ok\sigma}^+ a_{ok\sigma} \right> = \frac{1}{2} \left[ 1 - \frac{\tilde{\epsilon}_{\alpha}(k)}{E_{\alpha}(k)} \tanh \frac{E_{\alpha}(k)}{2k_B T} \right],
\]

\[
\left< a_{\alpha'k\uparrow} a_{\alpha'k\downarrow} \right> = -\frac{\Delta_{\alpha}}{2E_{\alpha}(k)} \tanh \frac{E_{\alpha}(k)}{2k_B T}.
\]

Here \(n_{\alpha}\) is the average number of electrons per site and \(\Delta_{\alpha}\) is the superconductivity gap in the orbital \(\alpha\); \(N\) is the number of lattice sites;

\[
\tilde{\epsilon}_{\alpha}(k) = \epsilon_{\alpha}(k) + \frac{1}{2} U_{\alpha\alpha} n_{\alpha} - \mu;
\]

\[
\epsilon_{\alpha}(k)\]

is the electron band energy associated with the orbital \(\alpha\) and

\[
E_{\alpha}(k) = \sqrt{\tilde{\epsilon}_{\alpha}(k)^2 + |\Delta_{\alpha}|^2}.
\]

The superconducting phase transition temperature \(T_c\) is determined by the condition for the existence of non-trivial solutions of the system of equations (3) in the asymptotic limit \(\Delta_{1,2} \to 0\).

We carry out the numerical calculations for two-dimensional square lattice with hopping integrals between nearest neighbours \(t_{ij} = t\) and electron band energies associated with \(s\)-orbitals \(\epsilon_{\alpha}(k) = \epsilon_{\alpha}^0 - 2t \sin(ak_x) \sin(ak_y)\), \(a\) is the lattice constant, and \(-\frac{\pi}{a} \leq k_{x,y} \leq \frac{\pi}{a}\). The intra- and interorbital interactions are chosen as \(U_{11}^0 = -1.5t\), \(U_{22}^0 = -2.5t\), \(|U_{12}^0| = |U_{21}^0| = 0.04t\), and the orbital energy \(\tilde{\epsilon}_{\alpha}^0 = 0\). In all calculations \(k_B = 1\).

The calculated dependency of superconducting phase transition temperature \(T_c\) on \(n = n_1 + n_2\) is depicted in figure 1 for different values of \(\tilde{\epsilon}_{\alpha}^0\). As expected, Van Hove singularity present in the middle of the bands \cite{11, 17, 18} is reflected in the case \(\tilde{\epsilon}_{\alpha}^0 = \tilde{\epsilon}_{\alpha}^0\) as a maximum in the \(T_c(n)\) for half filled system \((n = 1)\) where the chemical potential \(\mu\) passes this singular point. If \(\tilde{\epsilon}_{\alpha}^0 \neq \tilde{\epsilon}_{\alpha}^0\) the function \(T_c(n)\) passes two maxima. In the latter case the temperature dependencies of superconducting gaps for the values of \(n\) corresponding to the extremum points of \(T_c(n)\) are presented in the left column of figure 2. One can observe the substantial interband proximity effect if \(n = 1.10\) and the moderate one if \(n = 2.90\). For better clarity, the quasiparticles densities of states corresponding to the set of parameters in figure 2 are shown in figure 3.
Figure 1. The superconducting phase transition temperature $T_c$ vs $n = n_1 + n_2$ for two different $\varepsilon_1^0/t = 0$ and $2$, respectively. (a)-(c) denotes characteristic extremum points of the function $T_c(n)$: $n = 1.10, 2.57, 2.90$.

Figure 2. The temperature dependence of superconducting gaps for fixed site energies $\varepsilon_1^0/t = 2$ and $n = 1.10, 2.57, 2.90$, (a)–(c), respectively (on left side). The corresponding temperature dependencies of the Cooper pairs sizes $\xi_{pairs}$ (on right side).
Figure 3. Quasiparticles density of states at $T = 0$ for three cases as in figures 2a-c, respectively. Note, the composite structure of the superconducting gap in figures 3a and c.

3. Sizes of Cooper pairs
The sizes of Cooper pairs $\xi_{pair}$ are estimated from the wave functions of the Cooper pairs $\psi_\alpha(r)$:

$$\xi_{pair}(\alpha) = \sqrt{\frac{\int dr |\psi_\alpha(r)|^2 r^2}{\int dr |\psi_\alpha(r)|^2}} = \sqrt{\frac{\int dk |\nabla_k \psi_\alpha(k)|^2}{\int dk |\psi_\alpha(k)|^2}} ; \quad \alpha = 1, 2 \quad (8)$$

with

$$\psi_\alpha(k) = \frac{\Delta_\alpha \tanh \frac{E_\alpha(k)}{2k_B T}}{2 E_\alpha(k)}. \quad (9)$$

The right side of figure 2 shows the evolution of the sizes $\xi_{pair}(\alpha)$ with temperature for the same three characteristic band fillings $n$. For the comparison the temperature dependencies of the superconductivity gap and Cooper pair size in the case of single-orbital negative-$U$ Hubbard model is depicted in figure 4.

As a general observation, we notice that if superconductivity in one band is prevailing, the size of the Cooper pair in the band with weaker superconductivity exhibits strong decrease with the rise of temperature from zero to $T_c$. Simultaneously, the decrease of the size of the Cooper pair in the band with stronger superconductivity is small. The most prominent example of such behaviour, in the two-orbital model, is depicted in figure 2a. Here the total number of electrons per lattice site $n = 1.10$ corresponds to the left maximum of $T_c$ in figure 1. The latter is caused by the vicinity of the chemical potential to the van Hove singularity (see figure 3a) of the band $\alpha = 2$ which strongly supports the intraband superconducting ordering there. As a result the behaviour of the size of the Cooper pair in the band $\alpha = 2$ is similar to the single-band situation.
with weak temperature dependence, c.f. figure 4. For the superconductivity in the band $\alpha = 1$, the intraband contribution is small and the superconducting ordering is mainly caused by the interband proximity effect leading to the strong temperature dependence of the Cooper pair size in this band. The number of electrons $n = 2.90$ corresponds to the right maximum of $T_c$ in figure 1. In this case the chemical potential is close to the van Hove singularity of the band $\alpha = 1$ (see figure 3c) resulting in the stronger decrease of the Cooper pair size in the band $\alpha = 2$ as one can see in figure 2c. For the value $n = 2.57$ the chemical potential position is far enough from the van Hove singularities of the both bands (see figure 3b). In this case, depicted in figure 2b, the gaps $\Delta_{1,2}$ are close and the Cooper pair sizes depend on temperature weakly.

4. Conclusion
We have established that in a two-orbital superconductor the sizes of the Cooper pairs can decrease with the temperature substantially stronger compared to the behavior in single-orbital system. The effect takes place in the band with weaker superconductivity due to the presence of interband proximity effect.

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