Interplay between spin-singlet and spin-triplet order parameters in a model of an anisotropic superconductor with cuprate planes

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Abstract. Model of a two-dimensional anisotropic superconductor with a relatively wide, partially filled conduction band is considered. Attractive nearest neighbor interaction with the amplitude \( V_1 \), and on-site interaction (with the amplitude \( V_0 \)) taken either as repulsive or attractive are included in the model, along with the tight-binding dispersion relation implying singularities in the density of states. The analytic study is based on the conformal transformation method, which can be regarded as an extension of the Van Hove Scenario, plausible for anisotropic systems such as high-\( T_c \) cuprates. Employing the Fourier harmonics as a complete and orthogonal basis for irreducible representations of the cuprate plane symmetry group (\( C_{4v} \)), the symmetry of the superconducting order parameter is identified for various values of the model parameters. A wide range of parameters \( \eta = 2t_2/t_1 \) (the ratio of the second and the first nearest neighbor hopping integrals) and \( n \) (the carrier concentration) is studied. The obtained diagrams allow one to identify and mark the areas of stability for the superconducting spin-singlet \( s \)- and \( d \)-wave and the spin-triplet \( p \)-wave order parameters. In particular the problem of coexistence of the \( s \)-, \( p \)- and \( d \)-wave order parameters is addressed and solved for selected values of the ratio \( V_0/V_1 \). A possible island of stability of the \( d \)-wave order parameter in the \( s \)-wave order parameter environment for a relatively strong on-site interaction is revealed. The triple points, around which the \( s \)-, \( d \)-, and \( p \)-wave order parameters coexist, are identified on the diagrams. It is shown that results of the calculations performed for the two-dimensional tight-binding band model are dissimilar with some obtained within the standard BCS-type approximation. The influence of the on-site interaction on the stability of the \( s \)-wave order parameter is explained in detail. The developed and widely illustrated formalism can be easily applied to some more composed models.

1. Introduction
In spite of the fact that it has been already over twenty years since the discovery of high-\( T_c \) superconductors, they still attract attention due to their unusual properties at relatively high temperatures. In particular, recent solid state implementations of quantum information processing take advantage of these properties allowing one to define the superconducting two-level system (qubit)
either on charge or on phase degrees of freedom [1,2]. In theoretical description of high-$T_c$ superconducting copper-oxides, one usually treats the carriers within the CuO$_2$ planes as a quasi-two-dimensional system of fermions [3-5]. This is due to the characteristic, strongly anisotropic and layered structure of these materials with the symmetry of the CuO$_2$ planes corresponding to the point group C$_4$ [6-8].

Assuming that, in general, a superconducting system can be described by an effective Hamiltonian with a given dispersion relation $\xi_k$ and anisotropic pairing interaction $V(k,k')$, one can derive the two fundamental equations for high $T_c$ superconductors: the gap equation

$$
\Delta_k = \frac{1}{N} \sum_{k'} V(k,k') \frac{\Delta_{k'}}{E_{k'}} \tanh \frac{E_{k'}}{2T},
$$

where $E_k = \sqrt{\left(\xi_k - \mu\right)^2 + \Delta_k^2}$, and the equation

$$
2n = \frac{1}{N} \sum_k \left(1 - \frac{\xi_k - \mu}{E_k} \tanh \frac{E_k}{2T}\right),
$$

which allows one to determine the total chemical potential $\mu = \mu_0 + \mu(T)$ for a given conduction band filling $0 < n < 1$ fixed for the normal metallic phase at $T = 0$. Here $\mu_0$, defined for the metallic phase at $T = 0$, fixes the shift of the Fermi level due to doping, whereas $\mu(T)$ is the temperature correction.

The experimental data and studies of the electron-phonon interaction in strongly correlated superconducting cuprates within the $t$-$J$ model supply a direct evidence of a phonon contribution to the pairing interaction [9], similarly to the mixed phononic and electronic model, where the phononic pairing occurs between holes strongly dressed by antiferromagnetic fluctuations [4]. However, we have to emphasize that there are also some other approaches where the pairing mechanism can be of magnetic origin, as in the magnetic interaction model which is mathematically analogous to the conventional electron-phonon problem with the generalized magnetic susceptibility playing the role of the phonon propagator [3]. Moreover, according to the idea of the tight binding description one can assume that the overlap of the orbitals in different unit cells is small compared to the diagonal overlap values. Thus the matrix element of the pairing interaction $V(k,k')$ may contain the on-site, the nearest neighbors and the further neighbors terms, which give rise to diverse wave-symmetry channels [10].

This paper is aimed to point to a possibility of realization of a spin-singlet (i.e. $S = 0, M = 0$) $d$-wave symmetry state or a spin-triplet (i.e. $S = 1, M = 0$) $p$-wave symmetry state. The results presented here, allow us to define stable regions of the order parameter for given values of model parameters, and identify some potentially global conditions of realization and coexistence of distinct superconducting states with a fixed symmetry.

2. Model

Let us consider a system with a dispersion relation of the tight-binding band model

$$
\xi_k = -2t_0 \left(\cos k_x + \cos k_y + \eta \cos k_x \cos k_y\right)
$$

where $\eta = 2t_1/t_0 < 1$ and $t_0$, $t_1$ denote the nearest-neighbor and the next-nearest-neighbor hopping integrals, respectively.

The boson-mediated pairing interaction corresponding to on-site and nearest-neighbors pairing allows one to obtain the attractive interaction in the reciprocal space as [11,12]
where $V_0, V_1 > 0$ are the amplitudes of the isotropic and the anisotropic channel, respectively. The interaction (4) can be expressed as $V(k, k') = V^s(k, k') + V^t(k, k')$, where $V^s(k, k')$ and $V^t(k, k')$ are the spin-singlet and the spin-triplet pairing potentials, respectively. The pairing interaction is assumed to be strongly anisotropic in both spin-symmetric and spin-antisymmetric channels. The maximal boson energy $\omega_c$ is identified with the cut-off parameter imposed on the one particle energy: $-\omega_c \leq \xi \leq \omega_c$. The assumed form (4) of the interaction is sufficiently general to allow us to derive stable superconducting states from the spin-singlet and the spin-triplet ones, taking into account the s-wave and the d-wave symmetry states, as recognized in high-$T_c$ superconductors [6-8,13]. Below we focus on the anisotropic (forward scattering) interaction, which has a very rich structure and is responsible for d-wave symmetry pairing. Within the applied formalism we are also able to explain the role of the on-site interaction in creation of stable superconducting states [5,11-12]. In the following section we will briefly overview an analytical approach, which can be employed to extract the essential features of the discussed model.

3. Conformal transformation method

Recently, we have developed a formalism based on the conformal transformation of the momentum space, which can be treated as an extension of the standard Van Hove Scenario (VHS) [14]. In the standard VHS the summation over momenta $k$ (cf. equations (1) and (2)) is replaced by the integration over the particle energy $\xi$ and large values of the transition temperature are attributed to singularities or narrow maxima in the density of states (DOS) function $\nu(\xi) = 4\pi^{-2} \int df |\nabla_k \xi|^{-1}$ ($df$ is an element of the Fermi surface), corresponding to flat regions of the dispersion relation, where $\nabla_k \xi = 0$. The proposed approach [14] overcomes a weakness of the standard VHS which is the reduction of the number of degrees of freedom in a two-dimensional space only to one, namely the particle energy $\xi$. The main idea [14] of the conformal transformation method is to construct a new orthonormal 2D space $(\xi, \phi)$ in which $\xi$ stands for one of the coordinate axes. Hence, in this method the actual number of degrees of freedom is employed. The conformal transformation $(k_x, k_y) \mapsto (\xi, \phi)$ introduces local changes of the DOS in the $(\xi, \phi)$ space described by the Jacobian $J(\xi, \phi) = \left| \frac{\partial(k_x, k_y)}{\partial(\xi, \phi)} \right|$. Moreover, the coordinate $\phi$ can be identified with the angular variable $0 \leq \phi < 2\pi$ of the standard polar coordinate system. If any additional transformations are performed, the effective Jacobian is a product of Jacobians of successive transformations. Therefore, replacing the summation over the momentum in equations (1) and (2) by the integration over the particle energy, one has to include also the integration over the angle $\phi$ with the Jacobian $J(\xi, \phi)$. Only in the case when the integrand does not depend on the angle $\phi$ (e.g. for s-wave pairing) the summation can replaced by the integration solely over the particle energy with the DOS defined as $\nu(\xi) = \int_0^{2\pi} d\phi (2\pi)^{-1} K(\xi, \phi)$, where $K(\xi, \phi) = 2\pi^{-2} J(\xi, \phi)$ is the kernel of the DOS. Hence the standard VHS cannot be successfully applied to other than the pure s-wave pairing [14]. It is worth to emphasize at this point that the conformal transformation method allows one to study analytically many thermodynamic characteristics such as e.g. the critical temperature, specific heat or isotope exponent in a consistent and systematic manner [14]. Similar formalism has been also used very recently to study Fermi liquid instabilities in two-dimensional lattice models [15].
4. Interplay between spin-singlet and spin-triplet superconductivity

Performing the conformal transformation for the discussed model, we can re-express the gap equation (1) and the equation for the chemical potential (2) in terms of the variables $\xi$ and $\varphi$. The conformal transformation method offers all the advantages of the polar coordinate system $(\xi, \varphi)$. For the system under discussion, characterized by the dispersion relation (3), the kernel of the DOS can be found explicitly [6-18, 13]. Moreover, the basis functions of irreducible representations of the group $C_{4v}$, which is the symmetry group of the problem, can be chosen as the Fourier harmonics in the variable $\varphi$ [7]. Hence, the method allows one to expand the pairing potential (4), re-expressed in the new variables $(\xi, \varphi)$, in the double Fourier series. Both components (spin-symmetric and spin-antisymmetric) of the pairing potential (4) can be rewritten in terms of specifically chosen basis functions of irreducible representations of the group $C_{4v}$ [7]. If a single Fourier component dominates the others, the pairing potential for the corresponding state of pure pairing symmetry can be represented in the form given in table 1. Consequently, the order parameter has to be taken as

$$\Delta = \Delta_{l} = \Delta_{l}(\varphi)$$

and

$$\phi = \phi_{l}$$

where

$$\phi_{l} = \phi_{l}(\varphi)$$

is the averaged coefficient of the expansion of the pairing potential into the Fourier series [6, 7].

Table 1. Pairing potential for pure $s$-, $p$-, and $d$-wave pairing states. The coefficients $v_{l}(\xi; \eta, n) = \chi_{l}(\xi; \eta) / \overline{Z}_{l}(\eta, n)$, where $\overline{Z}_{l}(\eta, n) = (2\omega_{l})^{-1} \int_{-\omega_{l}}^{\omega_{l}} d\xi \chi_{l}(\xi; \eta)$ is the averaged coefficient of the expansion of the pairing potential into the Fourier series [6, 7].

| $l$ | Pairing potential |
|-----|-------------------|
| 0   | $-V_{0} - U_{0}(\eta, n) v_{0}(\xi; \eta, n) v_{0}(\xi'; \eta, n)$ |
| 1   | $-2U_{1}(\eta, n) v_{1}(\xi; \eta, n) v_{1}(\xi'; \eta, n) \left[ \cos \varphi \cos \varphi' + \sin \varphi \sin \varphi' \right]$ |
| 2   | $-2U_{2}(\eta, n) v_{2}(\xi; \eta, n) v_{2}(\xi'; \eta, n) \cos \varphi \cos \varphi' \left[ \sin \varphi \sin \varphi' \right]$ |

Replacing the summation over the momentum by the integration in the $(\xi, \varphi)$ space according to the conformal transformation method, one can rewrite the two fundamental equations (1) and (2) in the limit $T = T_c$ as [13]

$$1 = \left[ V_{0} \delta_{0,l} + U_{l}(\eta, n) \right] \frac{d\varphi}{2\pi} \int_{-\omega_{l}}^{\omega_{l}} d\xi K(\xi + \mu_{0}, \varphi; \eta) \frac{D_{l}^{2}(\varphi)}{\xi - \mu(\eta)} \tanh \frac{\xi - \mu(T)}{2T_c}$$

(5)

and

$$2n = \frac{1}{N} \left[ -\frac{d\varphi}{2\pi} \int_{-\omega_{l}}^{\omega_{l}} d\xi K(\xi, \varphi; \eta) \left[ 1 - \tanh \frac{\xi - \mu(\eta)}{2T_c} \right] \right]$$

(6)

where the functions $U_{l}(\eta, n) = V_{l} \overline{Z}_{l}^{2}(\eta, n)$ correspond to the coupling constant in the BCS-type factorizable pairing interaction [6-7] and it has been assumed that $v_{l}(\xi + \mu_{0}, n) \equiv 1$. On the other hand, employing equation (2) in the opposite limit ($T = 0$), we can find the relation among $n$, $\mu_{0}$ and $\eta$. It then turns out that the following symmetry relation holds $n(-\eta, \mu_{0}) = 1 - n(\eta, -\mu_{0})$ [7,8,13].

In order to identify the domains of stability for $s$-, $p$-, and $d$-wave superconducting states on the $(\eta, n)$ plane for chosen values of the ratio $\nu = V_{0}/V_{1}$, we compare the values of the transition temperature $T_{c}(l, n, \eta)$, found as a self-consistent solution of equations (5) and (6) [7-8,13]. According
to the experimental data, e.g. [16,17] (cf. also references in [14]), for cuprate materials $|\eta| < 0.9$, $t_0 = 0.24$ eV or 0.35 eV and $\omega_c$ takes values from 26 meV up to 65 meV. The numerical results presented in this section have been obtained for $\omega_c/2t_0 = 0.1$, and $\omega/\omega_c = 11$.

4.1. Critical temperature. BCS-type approximation
In order to provide a reference to our results it is instructive to calculate first the transition temperature within the standard BCS approach. Replacing the kernel of the DOS $K(\xi, \phi; \eta)$ by the standard DOS $\nu(\xi; \eta)$ and putting $v_1(\xi; \eta) \equiv 1$ one can reduce the gap equation (5) to the BCS-type form with the actual dimensionless pairing coefficients of the form $\nu_0(\eta)U_j(\eta)/2$, where the mean value of the DOS $\nu_0(\eta) = (2\omega_c)^{-1}\int_{-\infty}^{\infty} d\xi \nu(\xi; \eta)$. The critical temperature can be then found in a standard way as

$$
T_c(\ell, \eta, n) = \frac{2e^\gamma}{\pi} \omega_c \exp \left( -\frac{2}{\nu_0(\eta)U_j(\eta, n)} \right),
$$

(7)

where $\gamma$ is the Euler constant, or $T_c(\ell, \eta, n) = 0$ if $\nu_0(\eta)U_j + U_i(\eta, n) < 0$. The results obtained within the BCS-type approximation reveal a strong domination of the $s$-wave state in the presence of an attractive on-site interaction. Results of numerical calculations presented in figure 1 clearly illustrate

![Diagram](image)

**Figure 1.** The diagram of stable spin-singlet and spin-triplet superconducting states obtained within the BCS-type approximation: (a), $\nu = 0$ (b), $\nu = 0.5$ (c), $\nu = 0.6$, (d) $\nu \geq 0.64$. The half-filled band concentration ($\mu_0/2t_0 = 0$) is denoted by a dashed line. In figure (d) the equi-concentration lines are additionally displayed as thin dashed lines labelled with the values of the ratio $\mu_0/2t_0$ [8,13].
how the stability areas of the $s$-wave order parameter gradually dominate the diagram on the $(\eta, n)$ plane with increasing attractive on-site interaction. For $\nu \geq 0.64$, i.e. in the case of a strong attractive on-site interaction, only the $s$-wave order parameter survives (cf. figure 1d). On the other hand, in the case of a repulsive on-site interaction $\nu < 0$, our calculations [8,13] point out to the fact that the order parameter of the $s$-wave symmetry cannot be stable at all for $\nu < -0.61$. For moderate values of the parameter $\nu$ various symmetry states ($s$, $p$, and $d$-wave) can be observed (cf. figures 1a-c). In particular there exist some characteristic points on the $(\eta, n)$ around which the order parameters of the various symmetry can be realized. These points can be referred to as the ‘triple points’. Moreover, the symmetry relations for the carrier concentration mentioned at the beginning of the present section imply that for $l = 0, 1, 2$ we have $T_{\nu}[l, -\eta, n(-\eta, \mu_0)] = T_{\nu}[l, \eta, n(\eta, -\mu_0)]$ as reflected in the shape of the diagrams in figure 1 [8,13].

4.2. Critical temperature. Conformal transformation method
In order to derive the actual values of the transition temperature $T_c(l, n, \eta)$ within the tight-binding approach discussed in the present paper, we self consistently solve equations (5) and (6) using recently developed methods [7,8,13,14]. Note that also in this case the relation $T_{\nu}[l, -\eta, n(-\eta, \mu_0)] = T_{\nu}[l, \eta, n(\eta, -\mu_0)]$ holds for $l = 0, 1, 2$. The resulting diagrams are presented in figures 2 and 3. In these figures the supreme value of the superconducting transition temperature within the $d$-wave stability area is marked with a dotted line, which always goes through the origin of the coordinate system. The characteristic feature of the ‘triple’ points is also present in these diagrams (figures 2 and 3a-3c). The location of the triple points on the diagrams in figure 2 are presented in table 2.

| $\nu$ | 0     | 0.5   |
|-------|-------|-------|
| $(\eta, n)$ | (-0.75, 0.26) | (-0.24, 0.28) |
| $(\eta, n)$ | (0.75, 0.84) | (0.24, 0.72) |

Table 2. The location of triple points on the diagrams in figure 2 [8].

Figure 2. The diagram of stable spin-singlet and spin-triplet superconducting states obtained within the tight-binding approach: (a) $\nu = 0$, (b) $\nu = 0.5$. The half-filled band concentration ($\mu_0/2t_0 = 0$) is denoted by a dashed line [8,13].

From the diagrams in figure 2, and especially 3, we can conclude that the stability areas for the $s$-wave state expand, when the positive ratio $\nu$ of the pairing amplitudes increases up to the value 0.64.
Then the $p$-wave symmetry is eliminated from the diagram (cf. figures 3 a, b). Further increase in the ratio $\nu$ results in shrinking of the $d$-wave stability domain, which eventually forms an island occupying the central section of the diagram (figure 3c). Finally, when the ratio is greater than 0.9 the island vanishes and only the $s$-wave state is stable in the system (figure 3d). Again, in the case of a repulsive on-site interaction ($\nu < 0$), our calculations [8, 13] prove that the order parameter with the $s$-wave symmetry cannot be stable at all for $\nu < -0.61$.

5. Conclusions

In the present paper, employing the conformal transformation method [14], we have studied the interplay between the spin-singlet and spin-triplet order parameters, identifying the domains of stability for $s$-, $d$- and $p$-wave superconducting states on the diagrams in the variables $(\eta, n)$.

The location of stability regions (figure 1) implies that within the BCS-type approximation the $s$-wave state is preferred by the system for low concentration $n$ if $\eta < -0.4$ and for high concentration if $\eta > 0.4$. The $d$-wave symmetry is expected to be realized for sufficiently large $|\nu|$ and moderate $n$.

The other parts of the diagrams are occupied by the $p$-wave states. On the other hand the stability domains found in the tight-binding approach are distributed according to the following scenario (figures 2, 3): for low concentration $n$ if $\eta < -0.4$ and for high concentration if $\eta > 0.4$ the spin-singlet $s$-wave state is the preferred one, as in the BCS-type approximation; the spin-triplet $p$-wave symmetry dominates in two separated areas. However now, the $d$-wave state is realized for moderate values of $n$ and $\eta$. It is also worth to emphasize that the evolution of the diagrams with the increasing ratio $\nu$ of the pairing amplitudes in these two cases is different. In the BCS-like approximation the $p$-wave state coexist with the $s$-wave in the final stage of the evolution (large values of $\nu$), whereas in the tight-binding approach it is the $d$-wave symmetry which forms an ‘island’ in the $s$-wave environment.

Figure 3. Evolution of a $d$-wave stability ‘island’ on the diagrams of spin-singlet and spin-triplet superconducting states obtained within the tight-binding approach: (a) $\nu = 0.6$, (b) $\nu = 0.7$, (c) $\nu = 0.85$, (d) $\nu \geq 0.9$. The half-filled band concentration ($\mu_0/2t_0 = 0$) is denoted by a dashed line. In figure (d) the equi-concentration lines are additionally displayed as thin dashed lines labelled with the values of the ratio $\mu_0/2t_0$ [8, 13].

Regarding the characteristic feature of triple points and coexistence of states with various symmetry of the order parameter, we can state that since all the diagrams have been evaluated in the limit $\Delta(T) \rightarrow 0$, the pure-symmetry states exist only in areas, which are separated from each other by phase transition lines (cf. Figures 2, 3a-3c). However, one can expect that in the superconducting phase, if the temperature $T$ is very close to $T_c(l, n, \eta)$, the phase transition lines broaden proportionally.
to $|T - T_c(l,n,\eta)|$. Then it is possible to find regions along the phase transition lines, where the orders parameters of various symmetry could coexist.

We do not insist that the results obtained within the tight-binding model are quantitatively complete. Our aim was rather to show that applying the presented method to some other more complex models of high-$T_c$ superconductors, one should obtain qualitatively comparable results. In particular, the triple point effect and coexistence of various symmetries of the order parameter should be possible to observe. Certainly, one can not expect that the model parameters $(n,\eta,\nu)$ can be covered in their full range discussed in this paper by a single superconducting system. There are however many possibilities in the experimental search for the discussed effects. The most promising candidates seem to be doped superconducting compounds such as spinel- and perovskite-type structures of the type $A_{2-y}B_yCuO_{4-x}$ and $A_yB_{3-x}Cu_{3}O_{6+x}$, where $A$ is a trivalent rare-earth and $B$ is a divalent alkali earth ion or organic superconductors with a controlled bandwidth and band-filling (cf. [13] and references therein).

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