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On Possibility of Realization of *d*- or *p*-Wave Symmetry States in Anisotropic Superconductors

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We consider a model of high-T_c superconductors with an anisotropic boson-mediated pairing mechanism corresponding to the nearest-neighbor interactions, and the one-particle dispersion relation characterized by 2D Fermi surface nesting. Based upon the tight-binding or $t-J$ approaches with half-filling we show that the effective pairing potential coefficients and the dispersion relation, which can be characterized by the parameter $\eta = 2t_1/t_0$, have a diverse and mutually competing influence on the values of transition temperatures. The spin-singlet *d*-wave symmetry superconducting state is realized for small values of η, whereas for sufficiently large values, the spin-triplet *p*-wave symmetry superconducting state should be formed. The specific heat jump and the isotope shift, as functions of the parameter η, are evaluated for the *d*- and *p*-wave symmetry.

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1. Introduction

In present theoretical investigations of high-T_c superconductors it is accepted that they should be considered as quasi-2D, strongly anisotropic systems of fermions [1–3]. In some more composed approaches superconductivity is considered as a mixture of coexisting local pairs and itinerant fermions coupled via a charge exchange mechanism [4, 5], or additional terms of energy are included, such as the formation energy of the Zhang–Rice singlet [6] or the Peierls phase factor, responsible for the diamagnetic response of the system [7]. Such approaches, which find their origin in a proposed model of the anisotropic Fermi liquid [8], allow us to reveal various types of superconducting behavior. However, in general, one can assume that any superconducting system can be described in terms of an effective Hamiltonian with a given one-particle dispersion relation $\xi_{\boldsymbol{k}}$, which should be compatible with experimental data [8, 9] and the anisotropic pairing potential $V(\boldsymbol{k}, \boldsymbol{k}')$. Then, after employing the Green function formalism, one can obtain in a self-consistent manner the two basic equations: the gap equation in the momentum space

$$\boldsymbol{\Delta}_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} V(\boldsymbol{k}, \boldsymbol{k}') \frac{\boldsymbol{\Delta}_{\boldsymbol{k}'}}{E_{\boldsymbol{k}'}} \tanh \frac{E_{\boldsymbol{k}'}}{2T}, \tag{1}$$

where $E_{\boldsymbol{k}} = \sqrt{(\xi_{\boldsymbol{k}} - \mu)^2 + \boldsymbol{\Delta}_{\boldsymbol{k}}^2}$, and the following equation:

$$2n = \frac{1}{N} \sum_{\boldsymbol{k}} \left(1 - \frac{\xi_{\boldsymbol{k}} - \mu}{E_{\boldsymbol{k}}} \tanh \frac{E_{\boldsymbol{k}}}{2T} \right), \tag{2}$$

where N denotes the total number of lattice sites. Equation (2) gives the chemical potential $\mu(T)$ as a function of the temperature and the conduction band filling $0 < n < 1$ fixed for the normal metallic phase at $T = 0$. The chemical potential $\mu(T = 0)$, which allows us to control the carrier concentration n, in the case of half-filling is equal to zero [7, 8, 10–13]. Since the conventional phonon-mediated pairing mechanism raises doubts, we assume a generic, boson-mediated, strongly anisotropic attraction mechanism providing pairing interaction in the spin-antisymmetric and the spin-symmetric channels [1, 3, 11]. Moreover, symmetry elements of quasi-2D superconducting systems correspond to the group C_{4v} [14, 15].

We claim that in systems, characterized in such a way, the realization of both the spin-singlet d-wave symmetry state ($S = 0,\ M = 0$) and the spin-triplet p-wave symmetry state ($S = 1,\ M = 0$) is possible. In order to substantiate our statement we consider the tight-binding model, which allows us to carry out detailed analytical and numerical calculations. The dispersion relation for the 2D one-band tight-binding model or for the $t{-}J$ model derived within the quantum Monte Carlo method, after performing changes of the momentum space variables, can be written as

$$\xi_{\boldsymbol{k}} = -2t_0(\cos k_x + \cos k_y + \eta \cos k_x \cos k_y), \tag{3}$$

where $\eta = 2t_1/t_0$ and the case $\eta = 0$ corresponds to the ideal nesting. The parameters $t_0,\ t_1$ are identified with the nearest-neighbor and the next-nearest-neighbor hopping integrals, respectively [16].

On the other hand, the boson-mediated pairing mechanism corresponding to the nearest-neighbor interactions allows us to obtain the attractive interaction in the reciprocal space in the form (here $a_x = a_y = 1$) [3, 17–19]:

$$V(\boldsymbol{k}, \boldsymbol{k}') = -V_1[\cos(k_x - k'_x) + \cos(k_y - k'_y)], \tag{4}$$

with the anisotropic channel amplitude $V_1 > 0$. The potential (4) can be rewritten as a sum of the spin-singlet $V^{\mathrm{s}}(\boldsymbol{k}, \boldsymbol{k}') = V^{\mathrm{s}}(-\boldsymbol{k}, \boldsymbol{k}') = V^{\mathrm{s}}(\boldsymbol{k}, -\boldsymbol{k}')$ and the spin-triplet $V^{\mathrm{a}}(\boldsymbol{k}, \boldsymbol{k}') = -V^{\mathrm{a}}(-\boldsymbol{k}, \boldsymbol{k}') = -V^{\mathrm{a}}(\boldsymbol{k}, -\boldsymbol{k}')$ components [14].

Moreover, the maximal boson energy ω_{c} is identified with the cut-off parameter imposed on the one-particle energy, $-\omega_{\mathrm{c}} \le \xi_{\boldsymbol{k}} \le \omega_{\mathrm{c}}$. Therefore, a high-$T_{\mathrm{c}}$ superconductor is considered as a metallic system with a narrow, half-filled conduction band of the width $2\omega_c$, and the pairing interaction covering the whole conduction band.

2. Formalism and results

In the present calculations we employ the extended Van Hove scenario (VHS) method [8, 11, 9] and show that the basic Eqs. (1) and (2), after a sequence of curvilinear transformations of the $\boldsymbol{k}$-space can be formulated in polar coordinates ξ (the quasiparticle energy) and φ, accompanied by the kernel of the density of states $\mathcal{K}(\xi, \varphi)$. The spatial structure of the order parameter is determined by a predominant coefficient of the expansion of the pairing potential in the double Fourier series.

First, applying the BCS-type approximation we assess the transition temperatures $T_{c0}(l, \eta)$ for the actual pairing coefficients $U_l(\eta)$ for $l = 0, 1, 2, 4$ [14, 15]. The forms of the actual pairing coefficients and the transition temperatures are presented in Figs. 1a and c, respectively. In Fig. 1b, the reduced mean value of the density of states vs. the parameter η is displayed. The derived transition temperatures allow us to state that within the BCS-type approximation the d-wave state ($l = 2$) is preferred if exclusively spin-singlet pairs can be formed. On the other

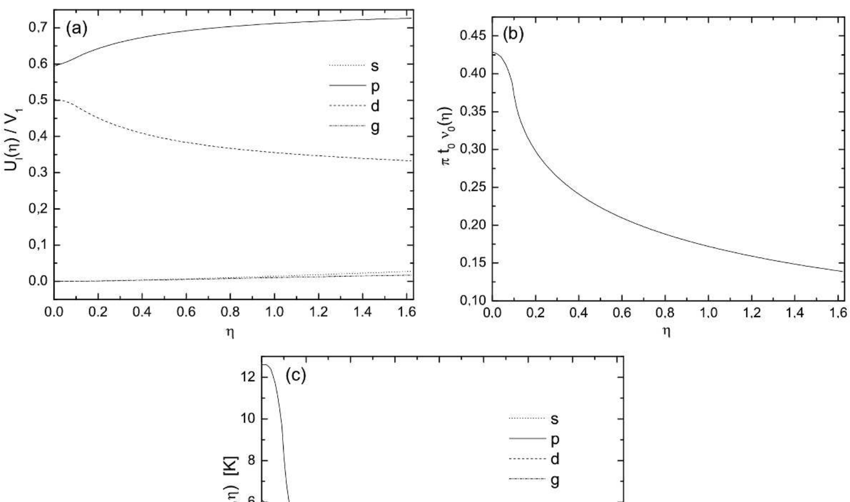

Fig. 1. The BCS-type approximation. (a) The relation between actual s-wave (dot), p-wave (solid), d-wave (dash), g-wave (dash-dot) symmetry pairing coefficients $U_l(\eta)$ and V_1 as functions of η ($0 < \eta \leq 1.62$). (b) The reduced mean value of the density of states $\pi t_0 \nu_0(\eta)$. (c) The transition temperatures $T_{c0}(l, \eta)$ for $V_1 = 2\pi t_0$ and $\omega_c \approx 560$ K.

hand, since $U_1(\eta) > U_2(\eta)$ for all values of η, the spin-triplet ($S = 1,\ M = 0$) p-wave state ($l = 1$) is the preferred one, in general. The spin-singlet isotropic s- and anisotropic g-wave states ($l = 0, 4$) cannot be realized because of their extremely low relative transition temperatures.

The formulae obtained within the extended Van Hove scenario [9, 15, 20] allow us to estimate some characteristic parameters of the superconductor as transition temperatures $T_c(l,\eta)$, the specific heat jump $\Delta C\,(T_c(l,\eta))$ and the isotope exponent $\alpha(l,\eta)$ as functions of η. Following the experimental data [21, 22], where one can find $\eta = 0.375$, 0.917, 1.055, 1.113 or 1.53, $t_0 = 0.24$ eV (≈ 2800 K), and $\omega_c = 0.026 \div 0.065$ eV, we can choose $\omega_c = 0.0048$ eV (≈ 560 K). In numerical evaluations we consider $0 < \eta \leq 1.62$, and we assume that the effective dimensionless pairing coefficient $\frac{1}{2}\nu_0(\eta)U_2(\eta) < 0.41$, which satisfies the weak-coupling condition, though the pairing coefficient V_1 can be large ($V_1 = 2.87$ eV), such that the standard dimensionless coefficient achieves the limit $\frac{1}{2}\nu_0(0)V_1 = 0.815$.

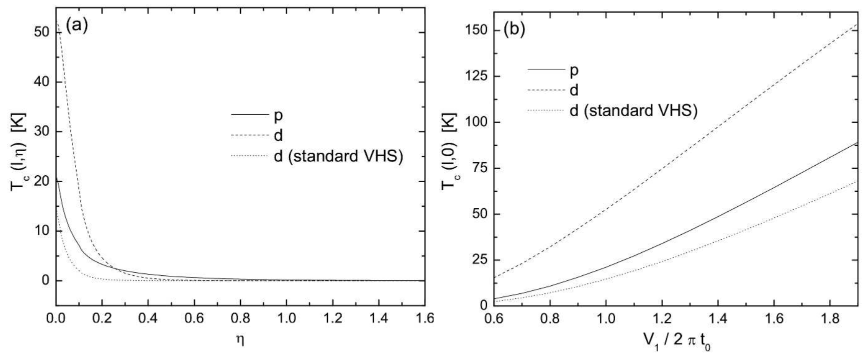

Fig. 2. (a) The transition temperatures $T_c(1,\eta)$ (solid) and $T_c(2,\eta)$ (dash) obtained within the extended VHS for $V_1 = 2\pi t_0$ and $V_0 = 0$ in comparison with the transition temperatures $T_c^*(2,\eta)$ (dot) obtained in the frame of the standard VHS. (b) Supreme values of the transition temperatures $T_c(1,0)$ (solid), $T_c(2,0)$ (dash), $T_c^*(2,0)$ (dot) for $0.6 \leq V_1/2\pi t_0 \leq 1.9$.

In Fig. 2 we present transition temperatures for p- and d-wave symmetry superconducting states. For $V_1 = 2\pi t_0 = 1.5$ eV, when $\frac{1}{2}\nu_0(0)U_2(0) = 0.215$, the supreme values of the transition temperatures $T_c(1,0) = 21.1$ K, $T_c(2,0) = 52.6$ K and $T_c(2,\eta) > T_c(1,\eta)$ for $0 < \eta < 0.256$. Moreover, $T_c(1,0.256) = T_c(2,0.256) = 2.47$ K, and $T_c(1,1.62) = 0.031$ K, $T_c(2,1.62) = 4.41 \times 10^{-6}$ K. Hence, in cuprates the d-wave symmetry superconducting state is realized for sufficiently small η. Instead, when η exceeds a characteristic value, the p-wave symmetry spin-triplet pairs should appear. The p-wave pairing becomes plausible when magnetic correlation effects in the CuO_2 planes determine the dispersion relation [1, 3]. Moreover, $T_c^*(2,\eta)$ obtained according to the standard Van Hove scenario, is lower than $T_c(2,\eta)$ and $T_c(1,\eta)$ for all η.

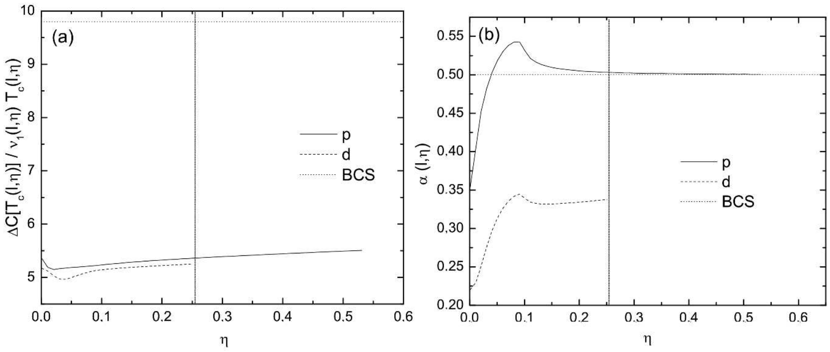

Fig. 3. (a) The reduced value of the specific heat jump at the transition temperature for p-wave (solid) and d-wave (dash) symmetry superconducting states plotted against the BCS-model value 9.38 (dot). In the limit $\eta \to 0$ they are equal to 5.35 and 5.17, respectively, though they are almost constant around 5.3 for all values of the parameter η under consideration. (b) The isotope shift $\alpha(l,\eta)$ for p-wave (solid) and d-wave (dash) symmetry superconducting states plotted against the BCS-model value 0.5 (dot). In the limit $\eta \to 0$ they are equal to 0.35 and 0.22, respectively. Let us note that the supreme value $\alpha(2, 0.091) = 0.345$ and for $\eta \geq 0.256$, $\alpha(1,\eta) \approx 0.5$.

In Figs. 3a and b we present the reduced specific heat jump at the transition temperature and the isotope shift $\alpha(l,\eta)$ for p-wave and d-wave symmetry superconducting states.

3. Conclusions

The obtained results evidence that the lack of the competition between singularities in the kernel of the density of states and pairing coefficients as in the BCS-type or standard Van Hove scenario approaches causes that the p-wave symmetry superconducting state dominates absolutely, since it corresponds to the largest absolutely coefficient $U_1(\eta)$. Thus, both the anisotropic attractive potential and dispersion relation have a crucial influence on values of the transition temperature. This result proves that, while considering a model of a superconductor with an anisotropic pairing potential, one has to include the kernel of the density of states $\mathcal{K}(\xi,\varphi)$ instead of the density of states $\nu(\xi)$ as e.g. in the standard Van Hove scenario [12, 20, 21, 23–28].

As distinct from some other approaches, where stability of superconducting states was investigated in dependence on the carrier concentration n for $\eta = 0$ [10], the obtained results delineate regions of stability of spin-singlet d-wave and spin-triplet p-wave superconducting states for $0 < \eta \leq 1.62$ and near to the half-filling, $n = 0.5$. These two types of approaches can be compared if $\eta = 0$ and $n = 0.5$, only, though both for large n and for large η, respectively, the stable d-wave state is replaced by the p-wave one.

Acknowledgments

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