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ANISOTROPIC PAIRING AND UNSCREENED LONG-RANGE INTERACTION IN HIGH-T_C SUPERCONDUCTORS

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Abstract. Recently observed anisotropy of the order parameter in high-T_c superconductors is explained by unscreened interaction of charge carriers with long-wave optical phonons.

Key words: superconductivity, superconducting gap, Coulomb interaction, s-wave, d-wave, pairing.

According to recent investigations the order parameter Δ (i.e. the gap) in high-T_c superconductors is strongly anisotropic (see e.g. [1,2]). Anisotropy is observed along ab plane, whereby maximal Δ values are in a and b directions ($\Gamma - M$ directions in $\vec{k}$-space) and the minimal ones, in between ($\Gamma - Y$ directions in $\vec{k}$-space). It is remarkable that the density of states at the Fermi surface has also the same anisotropy. At present it is not clear yet whether the sign of $\Delta(\vec{k})$ dependence is alternative or it remains positive for all directions. The recently-observed superlinear (cubic) dependence of Cu and O nuclear spin relaxation rate on temperature ($\gamma \sim T^3$) [3] and the intensity of electronic Raman scattering on frequency ($I \sim \omega^3$) [4] certify that the value of $|\Delta|$ near the Fermi surface in $\Gamma - Y$ direction is rather small in comparison with its value in $\Gamma - M$ direction.

The parameter $|\Delta|$ with the nodal line in $\Gamma - Y$ direction is characteristic of the angular momentum of Cooper pairs l=2 (s.c. d-wave pairing). Therefore, the experimentally-observed anisotropy of $|\Delta|$ is commonly considered as a strong support of those theoretical models which lead to the d-wave pairing. This applies especially to the models in which pairing interaction is caused by spin fluctuations (see, e.g. [5–8)], as high-T_c superconductors exhibit indeed strong antiferromagnetic (AF) fluctuations. Nevertheless, as long as sign-alternative behaviour of $\Delta(\vec{k})$ characteristic of the d-wave pairing has not been proved, the models leading to strongly anisotropic s-wave pairing (l=0) remain topical. The experimentally-observed reduction of the Knight shift below T_c [9] as well as the Josephson tunnelling between high-T_c and usual superconductors also support a singlet pairing.

Recently the authors of [10] proposed a model which allows to obtain a strongly anisotropic s-wave pairing. In this model pairing interaction arises from a Josephson-type pair tunnelling between the nearest CuO_2 planes. Below we propose another model which also leads to a strongly anisotropic s-wave pairing. In our consideration we take into account that anisotropic s-wave pairing may take place when pairing interaction has a long-range part. Indeed the superconducting gap results from the mixing of free-particle states near the Fermi surface by the interaction. Long-range interaction mixes the states with close $\vec{k}$ vectors and therefore it may lead to a $\vec{k}$-dependent gap Δ. The anisotropy of Δ in this case is of the same type as that of the density of states (ρ) on the Fermi surface while Δ increases with ρ. As we already mentioned above, this is just the situation in high-T_c superconductors.

In ordinary superconductors long-range Coulomb interactions are very weak due to their almost perfect screening by free charge carriers. However, in high-T_c superconductors these interactions are remarkable. Direct experimental evidences of that are given by renormalization of long wave vibration modes by superconducting transition observed in Raman and infrared spectra [11,12,13].

Usually the imperfect screening of long-range Coulomb interactions in high-T_c superconductors is associated with layered structure, relatively low charge carrier concentrations and low symmetry [14,15]. Notice that the large slow AF fluctuations observed in these materials also enhance the long-range Coulomb interactions. Indeed, these fluctuations are associated with the local lowering of the charge carrier concentration. Therefore, in AF-ordered clusters Coulomb interactions are not screened. The same holds for the areas in their vicinity up to the characteristic length of $\sim \lambda$, the penetration depth of the infrared field being associated with an optical phonon (the s.c. skin depth). At low (and probably intermediate) charge carrier concentrations λ essentially exceeds the n.n. Cu-Cu distance. Therefore nontotally screened areas overlap and, as a result, charge carriers interact remarkably with long-wave optical phonons. Note that charge carriers interactions with spin excitations of AF clusters should be weaker, as charge carriers and spin excitations of AF clusters are separated in space and their interaction is a short-range one.

According to the BCS mean field theory the quasiparticles spectrum is determined by the equation

$$\Delta_{\vec{k}} = -\sum_{\vec{k}'} U_{\vec{k}\vec{k}'} \chi_{\vec{k}'} \Delta_{\vec{k}'} , \qquad (1)$$

where $\chi_{\vec{k}} = (1/2E_{\vec{k}}) \tanh(E_{\vec{k}/T})$, $E_{\vec{k}} = (\Delta^2_{\vec{k}} + \varepsilon^2_{\vec{k}})^{1/2}$ determines the quasiparticle's energy, $\varepsilon_{\vec{k}}$ is the energy of a free single charge carrier measured from the Fermi energy ε_F,

$$U_{\vec{k}\vec{k}'} = \frac{\sum_\nu |g_\nu(q)|^2 \omega_{\nu\vec{q}}^2}{[(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'})^2 - \omega_{\nu\vec{q}}^2]} \tag{2}$$

is the interaction of the Cooper pairs arising from electron-phonon coupling, $\vec{q} = \vec{k} - \vec{k}'$, $\omega_{\nu\vec{q}}$ is the frequency of the phonon of the branch ν and the wave vector $\vec{q}$, $g_\nu(q)$ is the dimensionless interaction function ($\hbar = 1$, $k_B = 1$). We consider that this function has maximum at small q for which $\varepsilon_{\vec{k}} \approx \varepsilon_{\vec{k}+\vec{q}}$ and $U_{\vec{k}\vec{k}'} \approx U(\vec{k} - \vec{k}')$. In this case

$$\Delta_{\vec{k}} = \sum_{\vec{q}} U(q) \chi_{\vec{k}+\vec{q}} \Delta_{\vec{k}+\vec{q}} - \sum_{\vec{k}'} u_{\vec{k}\vec{k}'} \chi_{\vec{k}'} \Delta_{\vec{k}'} \;, \tag{1a}$$

where $U(q) = \sum_\nu |g_\nu^{(0)}(q)|^2$ allows for the maximum mentioned and $u_{\vec{k}\vec{k}'}$ stands for the rest of interaction which is the usual BCS interaction. We note that Eq. (1a) holds not only for a weak but also for a moderate and even a strong coupling with long wave phonons.

We suppose that the Fermi wave vector $\vec{k}_F$ is large in comparison with the q characteristic of $U(q)$. Then in (1a) for $\vec{k}$ near $\vec{k}_F$ $\Delta_{\vec{k}+\vec{q}} \approx \Delta_{\vec{k}}$ and the gap equation gets the form

$$\Delta_{\vec{k}} \approx \frac{-\sum_{\vec{k}\vec{k}'} u_{\vec{k}\vec{k}'} \chi_{\vec{k}'} \Delta_{\vec{k}'}}{(1 - \xi_{\vec{k}})}, \tag{3}$$

where

$$\xi_{\vec{k}} = \sum_{\vec{q}} (U(q)/2\vec{E}_{\vec{k}+\vec{q}}) \tanh(\vec{E}_{\vec{k}+\vec{q}}/T) \;, \tag{4}$$

$$\vec{E}_{\vec{k}+\vec{q}} \approx [\Delta^2_{\vec{k}_F} + (q_x E'_x(\vec{k}_F) + q_y E'_y(\vec{k}_F))]^{1/2} \;, \tag{5}$$

where $E'_{x,y}(\vec{k}_F) = dE_{\vec{k}}/dk_{x,y}$, $\vec{k} = \vec{K}_F$. Approximation (5) holds when the derivatives $E'_{x,y}$ do not diverge.

We suppose (contrary to [10]) that the tunnelling of the pairs between the nearest CuO_2 planes does not give any remarkable contribution to $\Delta_{\vec{k}}$ and restrict ourselves to the consideration of the pairs moving along CuO_2 planes. In this approximation in (3)-(5) $\vec{k}$ and $\vec{q}$ can be considered as two-dimensional vectors. Taking into account that for small q the unscreened interaction function $g(q) \sim q^{-1}$ and that in the case of a partial screening $g(0) \neq 0$, we can approximate $U(q)$ by the following formula

$$U(q) = U/(\kappa^2 + q_x^2 + q_y^2) \;, \tag{6}$$

where $\kappa << k_F$. Here $\kappa \equiv \kappa(c)$ depends on the hole concentration, c; this dependence is weak for small c (when the unscreened area is determined by an individual hole), but it is remarkable ($\kappa \sim c$) for higher hole concentrations. The $U(q)$ dependence (6) is in a qualitative agreement with experiment [16], where the maximal phonon renormalization by superconducting transition has been found for small q. Note that the condition $\kappa << k_F$ (and, on the whole, formula (6)) holds only in the case of intermediate charge carrier concentrations when k_F is not too small and κ is not too large.

By performing a rotation in $\vec{k}$ space at the angle $\alpha = \arccos(E'_x \rho)$ (which determines the direction of the normal vector to the Fermi surface at $\vec{k}_F$), where

$$\rho = ({E'_x}^2 + {E'_y}^2)^{-1/2} \tag{7}$$

is the density of states at the Fermi surface along α, one can integrate in (4) over $\tilde{q}_y = -q_x \sin\alpha + q_y \cos\alpha$ (here and below $E'_{x,y} \equiv E'_{x,y}(\varphi)$, $\rho \equiv \rho_\varphi$, $\xi \equiv \xi_\varphi$, and $\Delta \equiv \Delta_\varphi$ depend on the angle $\varphi = \arccos(k_{Fx}/k_F)$). Then for $\vec{k} \approx \vec{k}_F$

$$\xi \approx U \int_0^\infty dQ \tanh(E_Q/T)/E_Q \sqrt{Q^2 + \kappa^2}\,, \tag{8}$$

where $Q \equiv \tilde{q}_x = q_x \cos\alpha + q_y \sin\alpha$, $E_Q = (\Delta^2 + Q^2/\rho^2)^{1/2}$. At $T = 0$ this expression takes the form

$$\xi = U\rho \int_0^\infty \frac{dQ}{\sqrt{(Q^2 + \Delta^2\rho^2)(Q^2 + \kappa^2)}} = \frac{U\rho}{a} K(1 - b^2)\,, \tag{9}$$

where $K(x)$ is a full elliptical integral, $a = \kappa$, $b = \Delta\rho/\kappa$ if $\kappa > \Delta\rho$ and $a = \Delta\rho$, $b = \kappa/\Delta\rho$ in the opposite case.

Here we consider the weak coupling limit when $\kappa >> 2\Delta_\varphi\rho_\varphi$. In this case

$$\xi_\varphi = (U\rho_\varphi/\kappa)\ln(4\kappa/\Delta_\varphi\rho_\varphi)\,. \tag{10}$$

The contribution of the BCS interaction is as follows:

$$-\sum_{\vec{k}'} u_{\vec{k}\vec{k}'} \Delta_{\vec{k}'}/2E_{\vec{k}'} = V < \Delta_\varphi \ln(2\hbar\bar{\omega}/\Delta_\varphi) >\,, \tag{11}$$

where $\bar{\omega}$ is the mean phonon frequency,

$$V = < u_\varphi >\,,$$

$$< A_\varphi > = \int_F dk_F (u_\varphi/V)\rho_\varphi A_\varphi \tag{12}$$

is the averaging over the Fermi surface (integration in (12) has been performed along the Fermi surface). Here we take into account that $u_{\vec{k}\vec{k}'}$ describes a short-range interaction, due to which the sum in (11) does not depend on φ.

By substituting (10) and (11) into (3), one obtains the following integral equation for Δ_φ (T=0):

$$\Delta_\varphi(1 - (U\rho_\varphi/\kappa)\ln(4\kappa/\Delta_\varphi\rho_\varphi)) = V < \Delta_\varphi \ln(2\hbar\omega/\Delta_\varphi) > . \quad (13)$$

Let us consider two limiting cases: a) $U >> V$ and b) $U << V$.

a) In the first case φ-dependence of Δ is weak

$$\Delta_\varphi \approx \Delta[1 + (U\rho_\varphi/\kappa)\ln(4\kappa/\Delta_0\rho_\varphi)] . \quad (14)$$

Here

$$\Delta = \Delta_0(1+\delta) ,$$

$$\Delta_0 = 2\hbar\omega \exp(-1/V) \quad (15)$$

is the BCS gap (isotropic),

$$\delta = (U/\kappa V) < \rho_\varphi \ln(4\kappa/\Delta_0\rho_\varphi) > . \quad (16)$$

Δ_φ is larger in these directions where ρ_φ is larger.

b) In the second case ($U << V$)

$$\Delta_\varphi \approx \Delta_\varphi^{(0)} + \Delta^{(1)} , \quad (17)$$

where

$$\Delta_\varphi^{(0)} = (4\kappa/\rho_\varphi)\exp(-\kappa/U\rho_\varphi) \quad (18)$$

$$\Delta^{(1)} = V < \Delta_\varphi^{(0)} \ln(2\hbar\omega/\Delta_\varphi^{(0)}) > \quad (19)$$

($\Delta^{(1)} << \Delta_\varphi^{(0)}$). In this case the gap is strongly anisotropic; the larger values of Δ are in the directions in which ρ_φ is larger as well.

Symmetry of the function ρ_φ is determined by symmetry of the gradient of the Fermi surface in the $\vec{k}$-space. The energetical spectrum of free charge carriers (holes) in CuO_2 planes in high-T_c superconductors [7,10] is often described by the formula

$$\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \varepsilon_F , \quad (20)$$

where k_x and k_y correspond to the wave vector components in a a and b directions, $t \approx 0.25$ eV, $t' \approx 0.45\,t$ (see Fig.1). For $\varepsilon_F < -4t'$ the Fermi surface is closed around Γ point. In this case ρ_φ has maxima at

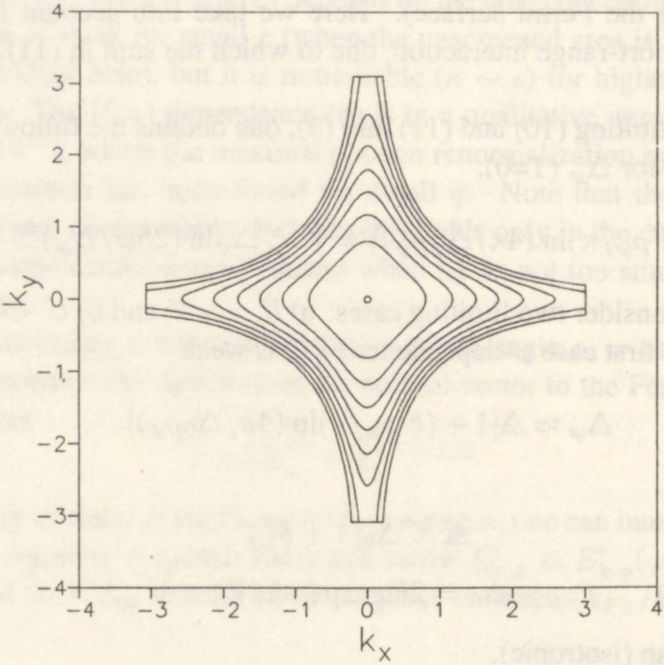

Fig. 1. The equienergetical lines $\varepsilon(k_x, k_y) = \varepsilon_F + \varepsilon_{\vec{k}}, \varepsilon_{\vec{k}} = -1.10001 + 0.03077$ k, k=0, 1, 2,...9; t=0.5.

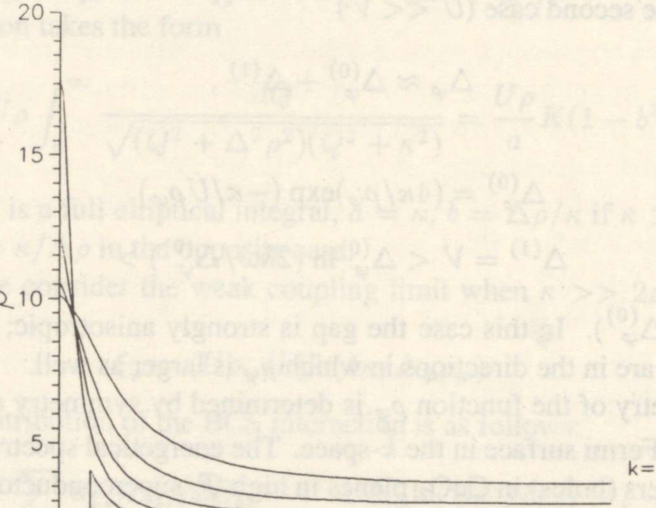

Fig. 2. The ρ (density of states) dependence on $\varphi = \arctan(k_x/k_y)$ for $\varepsilon_F = \varepsilon_{\vec{k}}$ (see Fig.1).

$\varphi = n\pi/2, n = 0,1,2,...$ (Fig.2). Such maxima were indeed observed experimentally [1]. According to obtained formulae (14)-(18), unscreened long-range interactions lead to anisotropy of the superconducting gap Δ_φ with maxima in the same directions. This result is in agreement with experiment. Finally we note that the critical temperature T_c is determined by maximum value of Δ_φ and ρ_φ (here at $\varphi = 0$). From Fig.2 one can see that ρ_0 is maximum for $\varepsilon_F \approx -4t'$. Consequently according to proposed model Δ_0 and T_c have maximum values at intermediate hole concentrations close to $\varepsilon_F \approx -4t'$. Such dependence of Δ on the doping concentration is also in a qualitative agreement with experiment.

We conclude that nontotally screened long-range electron-phonon interaction, which is observed in high-T_c superconductors, allows one to explain the anisotropy of the superconducting order parameter (gap) recently observed experimentally.

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ANISOTROOPNE PAARDUMINE JA EKRANEERIMATA KAUGMÕJU KÕRGTEMPERATUURSETES ÜLIJUHTIDES

Vladimir HIŽNJAKOV

Energeetilise pilu anisotroopiat kõrgtemperatuursetes ülijuhtides, mis hiljuti eksperimentaalselt avastati, on seletatud optiliste foononite ekraneerimata kaudmõjuga.

АНИЗОТРОПНОЕ СПАРИВАНИЕ И НЕЭКРАНИРОВАННОЕ ДАЛЬНОДЕЙСТВУЮЩЕЕ ВЗАИМОДЕЙСТВИЕ В ВЫСОКОТЕМПЕРАТУРНЫХ СВЕРХПРОВОДНИКАХ

Владимир ХИЖНЯКОВ

Обнаружунная недавно анизотропия энергетической щели в высокотемпераеурных сверхпроводниках объяснена не полностью экранированным взаимодействием носителей тока с оптическими фононами.