PHYSICA ⓒ

Towards the possibility of increasing T_c of oxide superconductors through coherent interaction of planar defects

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It is shown that the change in distance d between two linear defects in a two-dimensional superconductor can lead to the existence of periodical singularities $T_c \sim (d-d_n)^{-1}$ in the dependence of transition temperature on d; such singularities are the strongest among the ones known at present. The smoothing of these singularities is investigated with the following cutoff factors taken into account: inequality to zero of the coefficient of transmission through defects, quasiparticle attenuation, the finiteness of the temperature. The opportunity of raising T_c of oxide superconductors by inserting planar defects normal to the Cu–O planes is discussed.

1. Introduction

In the authors' recent paper [1] the existence of oscillations of the superconductor transition temperature, T_c, with a change in distance between two planar defects inserted in a superconductor was shown: this effect is similar to the effect of quantum oscillations which was observed in covered films [1–4] and was discussed by Kagan and Dubovsky [5]. According to ref. [1], to raise T_c one can use the coherent interaction of the planar defects; in the present paper this opportunity is discussed in relation to high-T_c oxide superconductors [6].

We assume that the BCS-type theory with coupling constant λ_0 and frequency cutoff ω_0 is valid for the oxide superconductors; it does not matter what the coupling mechanism between electrons (phonon, exciton and so on) is. Let us insert into the superconductors periodically repeated couples of planar defects, normal to the Cu–O planes: the distance d between defects in the couple is much smaller than a period L [#1], and $L \lesssim \xi_0$, where ξ_0 is the coherence length. Due to the planar defects the change in T_c

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[#1] On a qualitative level the obtained results are also valid in the case $d \sim L$. This is the simplest case for realization in experiment.

occurs. This change is defined by the following expression [7]:

$$\frac{\delta T_c}{T_{c0}} = \frac{1}{\lambda_0^3 L} V_0^2 \int dz \left[N_0 \, \delta N(z) + \delta N(z)^2 \right],$$

$$\delta N(z) = N(z) - N_0, \tag{1}$$

which is the exact consequence of the Gor'kov equations [7] for the case of localized space inhomogeneity; z-axis is normal to the plane defects, $N(z)$ is the local density of states at the Fermi level [4], integration is carried out over the interval including one couple of planar defects; T_{c0}, N_0 and V_0 are correspondingly transition temperature, the density of states and BCS interaction constant for the pure superconductor (we neglect the change of V near the planar defects). If we neglect the interaction between the Cu–O layers, we may consider a two-dimensional superconductor with linear defects.

In a three-dimensional superconductor containing planar defects with small transition coefficient the oscillations of the transition temperature have a sawlike form [1]: the system is divided by the defects into weakly coupled subsystems – films of thickness d_0 which have a quasicontinuous spectrum and the films of thickness d with a spectrum consisting of a set of 2D bands (fig. 1). If thickness d is increased, the distance between bands decreases; when the bot-
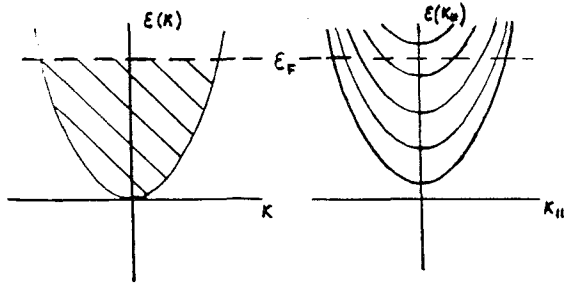
Fig. 1. When the coefficient of transmission through defects is small the system is divided by defects into weakly coupled subsystems of two types – films of thickness d_0 which have a quasi-continuous spectrum and films of thickness d with a spectrum consisting of a set of 2D-bands (on the right).

tom of some band intersects the Fermi level, T_c jumps up due to the jump of the density of states. In the two-dimensional case, 1D bands appear instead of the 2D ones in fig. 2. In the vicinity of the bottom of a 1D band the density of states depends on the energy ϵ as $\epsilon^{-1/2}$, so one can expect the appearance of periodical singularities $\sim (d-d_n)^{-1/2}$ in T_c. The periodical singularities do appear (fig. 2), but they are stronger than the ones discussed above, $T_c \sim (d-d_n)^{-1}$. The problem is that, in the intuitive arguments given above, we consider T_c of the space-inhomogeneous system as a function of the average density of states only (situation corresponding to the

Anderson theorem [9]). According to eq. (1), this is true in the case when in the integrand the first term is dominant (for example in the case $\delta N(z) \ll N_0$); the doubling of the singularity power is the consequence of the second term (in eq. (1)).

2. Form of T_c oscillations without cutoff of the singularities

Let the Cu–O layer lie in the plane $(y; z)$; separating the variables we get one-particle wave functions and eigenvalues E_n in the form

$$\Psi_n(y,z) = \varphi_s(z)\exp(ik_\parallel y) ,$$

$$E_n = \epsilon_s + k_\parallel^2/2m , \tag{2}$$

where $k_\parallel$ is the longitudinal quasimomentum and s is the transversal quantum number. It is supposed that the two-dimensional spectrum has the form $\epsilon(k) = k^2/2m$, and that linear defects have a negligible thickness in the transversal direction and are situated at the points $z = \pm d/2$ (according to eq. (1), it is enough to consider only one couple of defects). The boundary conditions for the wave function of traversal motion $\varphi(z)$ at point $z = d/2$ have the form
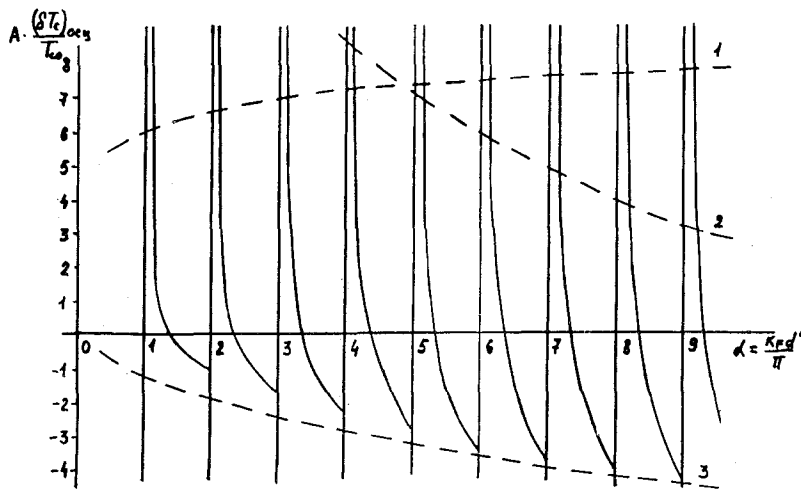
$$\varphi(d/2+0) = \varphi(d/2-0) ,$$

Fig. 2. Form of T_c oscillations with changing d (for $d=$const) without cutoff of the singularities; 1 and 2 are the envelopes of maxima when κ is finite (1) and l or T is finite (2); 3 – asymptotic form of the envelope of minima for the case $n \gg 1$.

$$\varphi'(d/2+0)-\varphi'(d/2-0)=\kappa\varphi(d/2),\qquad(3)$$

and at point $z=-d/2$ the conditions are analogous. Using the definition of the local density of states:

$$N(\epsilon,\mathbf{r})=\sum_n|\Psi_n(\mathbf{r})|^2\delta(\epsilon-E_n)$$

$$=\frac{\sqrt{2m}}{2\pi}\sum_s|\varphi_s(z)|^2\frac{\theta(\epsilon-\epsilon_s)}{\sqrt{\epsilon-\epsilon_s}},\qquad(4)$$

calculating $\varphi_s(z)$ and ϵ_s, transferring from summation by s to integration and neglecting terms $\sim a/L$ (a is the interatomic space), we get for $N(z)\equiv N(\epsilon_F; y, z)$:

$$N(z)=\frac{m}{\pi^2}\int_0^{k_F}\frac{dq}{(k_F^2-q^2)^{1/2}}$$

$$\times\begin{cases}\dfrac{2q^2}{\kappa^2}\dfrac{1+2q^2/\kappa^2+U_1(q)\cos 2qz}{V(q)}, & |z|<d/2,\\[2mm]\left[1+\dfrac{U_2(q)}{V(q)}\cos 2qz'+\dfrac{U_3(q)}{V(q)}\sin 2qz'\right],\end{cases}$$

$$z'=|z|-d/2>0,\qquad(5)$$

where

$$V(q)=(\sin qd+(2q/\kappa)\cos qd)^2+4(q/\kappa)^4,$$

$$U_1(q)=(2q/\kappa)\sin qd-\cos qd,$$

$$U_2(q)=-\sin^2qd-(2q/\kappa)\sin 2qd$$

$$+(2q^2/\kappa^2)(1-3\cos^2qd)+(2q^3/\kappa^3)\sin 2qd,$$

$$U_3(q)=(2q/\kappa)\sin^2qd+(3q^2/\kappa^2)\sin 2qd$$

$$+(4q^3/\kappa^3)\cos^2qd.\qquad(6)$$

The expected increase of T_c is large in the case of the strong defect, i.e. under condition $|\kappa|\gg k_F$. Below we shall discuss the case $\kappa\gg k_F$ only, because mean-field theory is not valid in the case $-\kappa\gg k_F$ [#2]. The expression for local density of states in the region $|z|<d/2$ can be transformed to

[#2] In the framework of mean-field theory in the vicinity of the linear defects, a localization of the order parameter occurs due to the existence of Tamm states, but in the case $d\gg a$ it is destroyed by fluctuations. Thus, in the two-dimensional case (in opposition to 3D), the existence of Tamm states has no qualitative effect and the results for the case $-\kappa\gg k_F$ should be similar to the ones for $\kappa\gg k_F$.

$$N(z)=\frac{m}{\pi^2}\int_0^{k_F}\frac{dq}{(k_F^2-q^2)^{1/2}}\frac{2q^2}{\kappa^2}$$

$$\times\frac{1-\cos 2qz\cos qd'}{\sin^2qd'+4q^4/\kappa^4}.\qquad(7)$$

It is clear that the integrand is localized near the points

$$q_n=\pi n/d',\qquad d'=d+2/\kappa,\qquad(8)$$

and one can approximate it by the set of δ-functions. The same situation occurs in the case $|z|>d/2$. One can get

$$N(z)$$

$$=\begin{cases}\dfrac{m}{\pi d'}\displaystyle\sum_{n=1}^M\dfrac{1-(-1)^n\cos 2q_nz}{(k_F^2-q_n^2)^{1/2}}, & |z|<d/2, & (9a)\\[3mm]N_0[1-J_0(2k_Fz')], & z'=|z|-d/2>0, & (9b)\end{cases}$$

where $N_0=m/2\pi$, $M=[k_Fd'/\pi]$, $J_0(x)$ is the Bessel function. According to eq. (9b), the integral over the region $|z|>d/2$ in eq. (1) does not depend on d and it may be calculated for $d=0$, i.e. for the case when two defects merge into one; the integral on the region $|z|<d/2$ gives the oscillational part of T_c:

$$\delta T_c(d)=\delta T_c(0)+(\delta T_c(d))_{\text{osc}}.\qquad(10)$$

Substituting eq. (9a) in eq. (1), we get ([...] – integer part of the number)

$$\frac{(\delta T_c)_{\text{osc}}}{T_{c0}}=\frac{1}{\pi\lambda_0}\frac{d'}{L}\left[-2S_1+\frac{4}{\pi}S_1^2+\frac{2}{\pi}S_2\right],$$

$$S_1=\sum_{n=1}^{[\alpha]}\frac{1}{(\alpha^2-n^2)^{1/2}},\qquad S_2=\sum_{n=1}^{[\alpha]}\frac{1}{\alpha^2-n^2},$$

$$\alpha=\frac{k_Fd'}{\pi}\qquad(11)$$

In the case when α is not very large, S_1 and S_2 consist of several terms and they are calculated straightforwardly; in particular, $(\delta T_c)_{\text{osc}}=0$ for $0<\alpha<1$. In the case $\alpha\gg 1$, one can express δT_c in terms of periodical functions $\psi(\{\alpha\})$ and $f(\alpha)$.

$$\frac{(\delta T_c)_{\text{osc}}}{T_{c0}}=\frac{1}{\pi\lambda_0 k_F L}$$

$$\times\left\{\ln 2\alpha - \psi(\{\alpha\}) + 2\pi\sqrt{\alpha}f(\alpha) + 4f^2(\alpha) - \pi\right\},$$

$$f(\alpha) = \sum_{n=1}^{\infty} \frac{\cos(2\pi n\{\alpha\}) - \pi/4}{\sqrt{n}}, \quad \alpha = \frac{k_F d'}{\pi},$$

$$(12)$$

where $\psi(z)$ is the logarithmic derivative of the gamma function [10], $\{...\}$ is the fractional part of the number. In the vicinity of the nth singularity we obtain in the leading approximation in n:

$$\frac{(\delta T_c)_{osc}}{T_{c0}}\bigg|_{\alpha \to n} = \frac{1}{\pi\lambda_0 k_F L}$$

$$\times\left\{2\pi f_{min}\sqrt{n} + \pi\sqrt{2n}\frac{\theta(\alpha-n)}{(\alpha-n)^{1/2}} + 3\frac{\theta(\alpha-n)}{\alpha-n}\right\},$$

$$(13)$$

where $f_{min} = -1.03$ is the minimum of the function $f(\alpha)$; the first term in brackets gives the envelope of the minima of the oscillations (fig. 2).

Substituting eq. (9b) in eq. (1), one can calculate the value of $T_c(0)$; the integral of $(\delta N)^2$ diverges logarithmically for large $|z|$. For dirty superconductors the cutoff distance is the electron mean free path l. The finite value of l may be taken into account by the substitution

$$\delta(\epsilon - E_n) \to \frac{1}{\pi}\frac{\gamma}{(\epsilon - E_n)^2 + \gamma^2}$$

$$(14)$$

in eq. (4), from which

$$\delta N(z) \to \delta N(z)e^{-2|z|/l}, \quad l = v_F/\gamma.$$

$$(15)$$

Calculating the integral in eq. (1) we get [#3]

$$\frac{\delta T_c(0)}{T_{c0}} = \frac{1}{\pi\lambda_0 k_F L}[\ln(4k_F l) - \pi].$$

$$(16)$$

In the case of a clean superconductor, the result for

[#] The derivation of eq. (1) for clean superconductors also remains valid in the dirty limit, but we must use the average $\langle K(z, z')\rangle$ instead of the kernel $K(z, z')$ (average is taken over impurity distribution). Instead of $N(z)$, the average quantity $\langle N(z)\rangle$ appears in eq. (1), which we can express in terms of the imaginary part of the average Green's function $\langle G(z; z')\rangle$. The quasiparticle attenuation is taken into account by the substitution $\epsilon \to \epsilon + i\gamma$, which is equivalent to eq. (14).

$\delta T_c(0)$ with logarithmic accuracy is obtained from eq. (18) by the substitution $l \to L$.

3. The cutoff of the singularities

Consider the main factors leading to the cutoff of the singularities.
(1) The finiteness of κ.
If κ is finite, then in the region $|z| < d/2$ we may write $N(z)$ in the form

$$N(z) = \sum_{n=1}^{\infty} A_n[1 - (-1)^n\cos 2q_n z],$$

$$(17)$$

where

$$A_n = \frac{m}{\pi^2}\int_{-q_n}^{k_F-q_n}\frac{dq}{(k_F^2 - (q_n+q)^2)^{1/2}}\frac{2q_n^2/\kappa^2}{(qd')^2 + 4q_n^4/\kappa^4}.$$

$$(18)$$

The singularities appear due to the Mth term of sum (17) ($q_M \approx k_F$). Separating this term and assuming $\kappa = \infty$ in the others, we obtain for T_c the expression

$$\frac{(\delta T_c)_{osc}}{T_{c0}}\bigg|_{\alpha \to n} = \frac{1}{\pi\lambda_0 k_F L}$$

$$\times\left\{2\pi f_{min}\sqrt{n} + \frac{2\pi^3 n}{m}A_M + \frac{6\pi^4 n}{m^2}A_M^2\right\}.$$

$$(19)$$

Calculating A_M for finite κ we get

$$\frac{(\delta T_c)_{osc}}{T_{c0}}\bigg|_{\alpha \to n} = \frac{1}{\pi\lambda_0 k_F L}$$

$$\times\left\{2\pi f_{min}\sqrt{n} + \pi^{3/2}\frac{\kappa}{k_F}\sqrt{n}F(u) + \frac{3\pi}{2}\frac{\kappa^2}{k_F^2}F(u)^2\right\},$$

$$u = \frac{\pi}{2}\frac{\kappa^2}{k_F^2}(\alpha - n),$$

$$(20)$$

where the function $F(u)$ describes the form of a smoothed singularity and is defined by

$$F(u) = \frac{1}{\pi}\int_0^{\infty}\frac{dx}{\sqrt{x}}\frac{1}{(u-x)^2 + 1}$$

$$= \frac{1}{\sqrt{2}}\left(\frac{u + (u^2+1)^{1/2}}{u^2+1}\right)^{1/2}.$$

$$(21)$$

Substituting $F(u) \to F_{\max} = (3/4)^{3/4} \approx 0.81$, one can obtain the envelope of the maxima.

(2) The quasiparticle attenuation.

The substitution (14) in eq. (4) takes into account the finiteness of the electron mean free path. In consequence one can obtain $N(z)$ in the form (17) with

$$A_n = \frac{1}{2\pi d'} \left(\frac{2m}{\gamma} \right)^{1/2} F\left(\frac{k_F^2 - q_n^2}{2m\gamma} \right), \tag{22}$$

and the function $F(u)$ is the same as that in eq. (21). Using eq. (19) we get

$$\left. \frac{(\delta T_c)_{\mathrm{osc}}}{T_{c0}} \right|_{\alpha \to n} = \frac{1}{\pi \lambda_0 k_F L}$$

$$\times \left\{ 2\pi f_{\min} \sqrt{n} + 2\pi \left(\frac{\epsilon_F}{\gamma} \right)^{1/2} F(u) + 6 \frac{\epsilon_F}{\gamma} \frac{1}{n} F(u)^2 \right\},$$

$$u = \frac{2\epsilon_F}{\gamma} \frac{\alpha - n}{n}. \tag{23}$$

The envelope of the maxima is obtained by the substitution $F(u) \to F_{\max}$. It is interesting that its dependence on n differs from eq. (20).

(3) The finiteness of the temperature.

When deriving eq. (1) in ref. [7], it was supposed that $N(\epsilon; z)$ changes slowly on the scale ω_0, and can be taken in the point $\epsilon = \epsilon_F$. Taking into account that $N(z)$ arises from the sum rule for the kernel,

$$\int K(r, r') \, dr' = N(r) N(r) \ln \frac{1.14\omega_0}{T}, \tag{24}$$

it is easy to understand that in the general case we must use

$$N_{\mathrm{eff}}(z) = \lambda_0 T \sum_s \int d\epsilon \frac{N(\epsilon, z)}{\epsilon^2 + \omega^2} \tag{25}$$

instead of $N(z)$, where summation is taken on Matsubara frequencies $\omega_s = \pi T(2s+1)$, ($|\omega_s| < \omega_0$); it is taken into account that $T \approx T_{c0}$. Transforming N_{eff} in the form (17), we get

$$A_n = \frac{\sqrt{2m}}{2\pi d'} \lambda_0 T \sum_s \int_0^\infty \frac{d\epsilon}{\sqrt{\epsilon}} \frac{1}{[\epsilon + (q_n^2 - k_F^2)/2m]^2 + \omega^2}. \tag{26}$$

If $\{\alpha\}/\alpha \gg \omega_0/\epsilon_F$ we return to eq. (13). In the opposite case, in accordance with eq. (19), we get

$$\left. \frac{(\delta T_c)_{\mathrm{osc}}}{T_{c0}} \right|_{\alpha \to n} = \frac{1}{\pi \lambda_0 k_F L}$$

$$\times \left\{ 2\pi f_{\min} \sqrt{n} + \frac{\pi \lambda_0}{\sqrt{2}} \left(\frac{\epsilon_F}{T} \right)^{1/2} G(u) \right.$$

$$\left. + \frac{3\lambda_0^2}{4} \frac{\epsilon_F}{T} \frac{1}{n} G^2(u) \right\},$$

$$u = \frac{\epsilon_F}{T} \frac{\alpha - n}{n}, \quad G(u) = \int_0^\infty \frac{dx}{\sqrt{x}} \frac{\mathrm{th}(x-u)}{x-u}. \tag{27}$$

The cutoff of the singularities occurs at $\{\alpha\}/\alpha \sim T/\epsilon_F$; in the interval $T/\epsilon_F \ll \{\alpha\}/\alpha \ll \omega_0/\epsilon_F$ the singularities have no pure power behavior due to logarithmic corrections. The function $G(u)$ describes the form of the maxima; we may obtain the envelope of maxima from eq. (27) by the substitution $G(u) \to G_{\max} \approx 3.8$.

4. Discussion of the results

From eqs. (20), (23) and (27) we obtain that the highest increase in T_c is reached under conditions

$$d \sim a, \quad \kappa \gtrsim k_F (\xi_0/a)^{1/2}, \quad l \gtrsim \xi_0, \tag{28}$$

and it has a value

$$\frac{\delta T_c}{T_{c0}} \sim \frac{\epsilon_F}{T_c} \frac{a}{L}. \tag{29}$$

If $L \sim \xi_0$, then we obtain $\delta T_c \sim T_{c0}$. If $\delta T_c \gtrsim T_{c0}$, the initial eq. (1) is not true, but from the physical sense one can expect further increase in T_c when L becomes smaller than ξ_0. The upper estimate (29) may not be reached because (1) the planar defects are not perfect; (2) in the vicinity of a singularity of the states the Fermi level is unstable [11], etc.

In the limit $\kappa \to \infty$, a two-dimensional superconductor is divided into 1D strips, in which superconductivity is destroyed by fluctuations. The fluctuations are not important if $J_\perp \gtrsim T$ [12] ($J_\perp$ is the transversal overlap integral). Substituting $J_\perp \sim \epsilon_F (\kappa a)^{-1}$ we get in the case $d \sim a$)

$$\kappa \lesssim k_F (\xi_0/a) \tag{30}$$

which is compatible with eq. (28).

One can create the considered structures (fig. 1) by the use of:

(a) the control of the twinning processes;

(b) the insertion of layers of alien atoms (*a*-oriented superlattices of the oxide superconductors with the period 100 Å already created [13]);

(c) deposition of thin films (about several Cu–O layers) on substrata with artificial periodicity.

It is interesting that the effect of increasing T_c occurs even in the case of random position of the planar defects (with the average distance L). Assuming that the distance d between defects fluctuates on the scale $\delta d\,(k_F^{-1} \ll \delta d \ll d, L)$ and taking the average of the eqs. (20), (23) and (27) by d in the interval from 0 to L, we get (taking into account eqs. (10) and (16)):

$$\frac{\delta T_c}{T_{c0}} = \frac{1}{\pi\lambda_0 k_F L}\left[3\ln\max\left\{\frac{\kappa^2}{k_F^2}, \frac{\epsilon_F}{\gamma}, \frac{\epsilon_F}{T}\right\}\right.$$

$$\left. + \ln\max(kl, kL) + \ln kd + 0(1)\right],$$

i.e. the estimate $\delta T_c/T \sim a/L$ is valid with a logarithmically large factor. This result is qualitatively valid if $\delta d \sim d \sim L$, when the occurrence of the defects is absolutely random. It is possible that the heightened T values which were irreproducibly observed in the beginning of the high-T_c superconductor investigation were stipulated by a high concentration of the planar defects or their mutual disposition.

Acknowledgement

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