Raising the critical temperature of the oxide superconductors

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It is shown that when the separation d between a pair of linear defects introduced into a two-dimensional superconductor is varied, periodic singularities in T_c of the form $T_c \propto (d - d_n)^{-1}$ arise; these are the strongest of the known singularities. The smearing of the singularities associated with various cutoff mechanisms is examined. These are (a) the finite transparency of the defects, (b) quasiparticle damping, and (c) finite temperatures. The introduction of plane defects perpendicular to the Cu–O layers is discussed as a possibility for significantly raising the T_c of the oxide superconductors.

1. INTRODUCTION

In a recent paper[1] we have predicted oscillations in the transition temperature T_c as a function of the distance d between two plane defects introduced into a superconductor; this effect is analogous to the quantum T_c-oscillations which have been observed on coated films[2–4] and discussed by Kagan and Dubovskiĭ.[5] We have shown[1] that one may exploit the coherent interaction between the plane defects as a means to enhance T_c; in the present paper this possibility is discussed for the high-temperature superconducting oxides.[6]

The oxide superconductor is assumed to be described by a BCS-type theory[1)] with a coupling constant λ_0 and a frequency cutoff ω_0; the precise nature of the electron-electron attraction mechanism (be it by phonons, excitons, or some other processes) is of no significance. As shown in Fig. 1, the superconductor in question contains a system of periodically repeated pairs of plane defects perpendicular to the Cu–O layers; the distance d between the defects of a given pair is small compared with the period L,[2)] and $L \lesssim \xi_0$, the coherence length. The change in T_c due to the presence of the plane defects is given by the expression[7]

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

$$\delta N(z) = N(z) - N_0 , \qquad (1)$$

which follows exactly from the Gor'kov equations[8] for a localized spatial inhomogeneity. Here the axis of z is normal to the defects; $N(z)$ is the local density of states at the Fermi level [cf. Eq. (4)]; the integration is carried out over a region containing one pair of defects; and T_{c0}, N_0, and V_0 represent the transition temperature, density of states, and the four-fermion interaction constant of the initial superconductor (we neglect changes in V_0 near the plane defects). Neglecting the interaction between the Cu–O layers reduces the problem to that of a two-dimensional superconductor with linear defects.

In a three-dimensional superconductor[1] when the defect transparency is low and $d_0 = \text{const}$, the oscillations of T_c with d are of a sawtooth shape. The reason for this is that the superconductor is divided by the plane defects into two types of weakly-coupled film subsystems, namely films of thickness d_0 whose spectrum is quasicontinuous and those of thickness d whose spectrum consists of a series of two-dimensional bands as shown in Fig. 2. Increasing d decreases the distance between the bands; each time the bottom of a two-dimensional band crosses the Fermi level of the system, a discontinuous increase in T_c occurs as a result of the jump in the density of states. In two dimensions, the two-dimensional bands go over to one-dimensional bands, with the property that the density of states near the bottom of a band depends on the energy as $\varepsilon^{-1/2}$; accordingly, periodic divergences $\sim (d - d_n)^{-1/2}$ may be expected in T_c. Now while

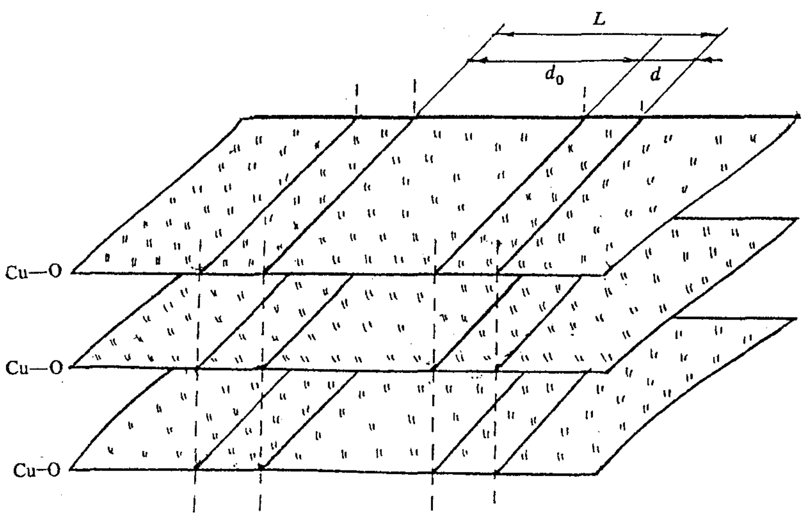

FIG. 1. The system under study is an oxide superconductor with paired plane defects introduced perpendicular to the Cu–O layers; d is the defect separation within a pair, L the pair separation.

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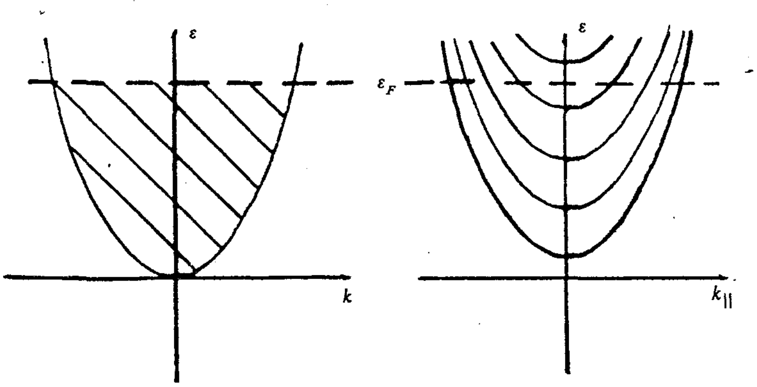

FIG. 2. For low defect transparencies the system decomposes into two weakly-coupled subsystems: films of thickness d_0 with a quasicontinuous spectrum (left) and those of thickness d, whose spectrum consists of a series of two-dimensional bands (right).

periodic divergences in T_c are indeed found (Fig. 3a), they turn out to satisfy $T_c \propto (d-d_n)^{-1}$—that is, the variation is stronger than expected. The reason is that in the intuitive argument above the T_c of a spatially varying system is considered as a function only of the average density of states (the situation for Anderson's theorem[9] to be valid); but this, according to (1), is only true if the integrand is dominated by its first term (e.g., when $\delta N(z) \ll N_0$); the extra factor of 2 in the exponent of the divergence is due to the second term in (1).

2. T_c OSCILLATIONS WHEN THE SINGULARITIES ARE NOT CUT OFF

If we let the Cu–O layer lie in the (y,z)-plane and separate variables, the one-particle wave functions $\Psi_n\,(y,z)$ and the eigenvalues E_n may be represented as

$$\Psi_n(y,z) = \varphi_s(z)\exp(ik_\parallel y), \qquad E_n = \varepsilon_s + k_\parallel^2/2m\,, \qquad (2)$$

where $k_\parallel$ is the longitudinal quasimomentum and s the transverse quantum number; it is assumed that the two-di-

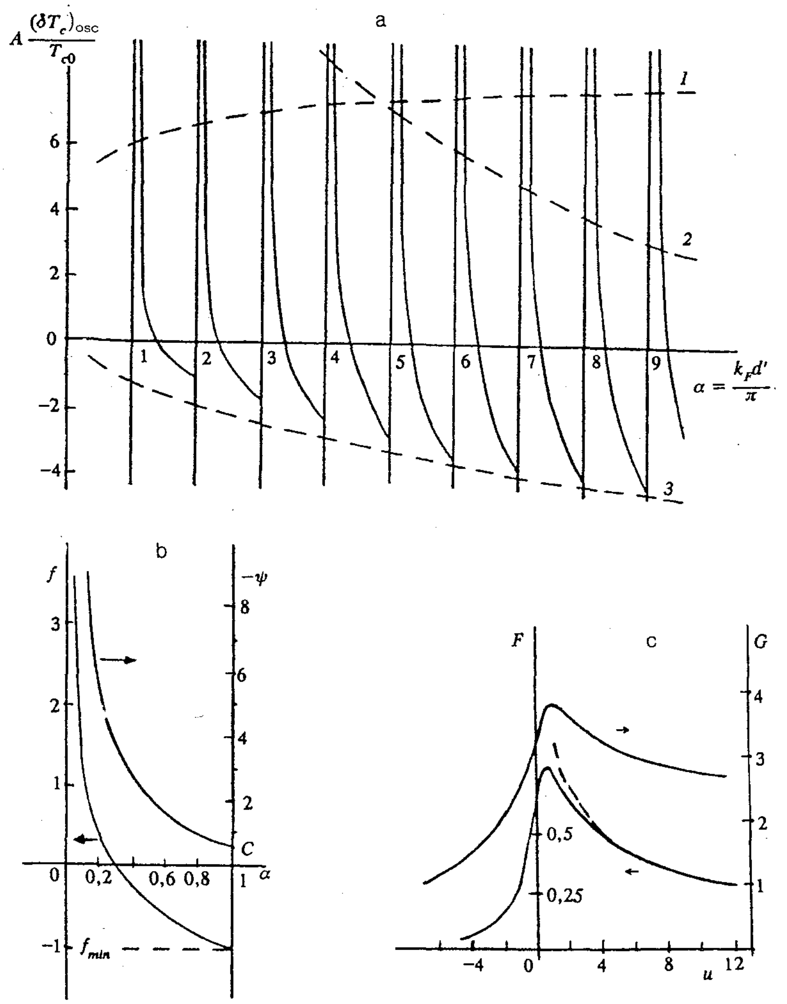

FIG. 3. (a) T_c oscillations with d in the absence of cutoff ($d_0 = \text{const}$); 1: the envelope of the maxima for singularities cut off due to the finite value of $\varkappa$: 2: the same for singularities cut off due to a finite quasiparticle lifetime or finite temperature; 3: asymptotics of the envelope of the minima for $n \gg 1$; (b) functions $\psi(\{\alpha\})$ and $f(\alpha)$ determining the shape of the oscillations for $n \gg 1$ within one period (C is Euler's constant); (c) functions $F(u)$ and $G(u)$ determining the shape of the smeared singularities; the dashed line: $F = u^{-1/2}$.

mensional spectrum is quadratic, $\varepsilon(k)=k^2/2m$, and that the linear defects are δ-functions in the transverse direction and are located at $z=\pm d/2$ [according to Eq. (1), only one pair of defects need be considered]. The boundary condition for $\varphi(z)$, the wave function for the transverse motion, may then be written as

$$\varphi\left(\frac{d}{2}+0\right)=\varphi\left(\frac{d}{2}-0\right),$$
$$\varphi'\left(\frac{d}{2}+0\right)-\varphi'\left(\frac{d}{2}-0\right)=\varkappa\varphi\left(\frac{d}{2}\right) \quad (3)$$

for $z=d/2$ and similarly for $z=-d/2$. Using the definition of the local density of states

$$N(\varepsilon,\mathbf{r})=\sum_n|\Psi_n(\mathbf{r})|^2\delta(\varepsilon-E_n)$$
$$=\frac{\sqrt{2m}}{2\pi}\sum_s|\varphi_s(z)|^2\frac{\theta(\varepsilon-\varepsilon_s)}{\sqrt{\varepsilon-\varepsilon_s}}, \quad (4)$$

calculating $\varphi_s(z)$ and ε_s and replacing the s summation by integration, we find, after dropping the terms $\sim a/L$, where a is the interatomic separation, that $N(z)\equiv N(\varepsilon_F;y,z)$ is given by

$$N(z)=\frac{m}{\pi^2}\int_0^{k_F}\frac{dq}{(k_F^2-q^2)^{1/2}}$$
$$\times\begin{cases}\dfrac{2q^2}{\varkappa^2}\dfrac{1+2q^2/\varkappa^2+U_1(q)\cos(2qz)}{V(q)}, & |z|<\dfrac{d}{2}\\[2ex] [1+\dfrac{U_2(q)}{V(q)}\cos(2qz')+\dfrac{U_3(q)}{V(q)}\sin(2qz')], & \end{cases}$$
$$z'=|z|-\frac{d}{2}>0, \quad (5)$$

where

$$V(q)=[\sin(qd)+\frac{2q}{\varkappa}\cos(qd)]^2+4\left(\frac{q}{\varkappa}\right)^4,$$
$$U_1(q)=\frac{2q}{\varkappa}\sin(qd)-\cos(qd), \quad (6)$$
$$U_2(q)=-\sin^2(qd)-\frac{2q}{\varkappa}\sin(2qd)$$
$$+\frac{2q^2}{\varkappa^2}[1-3\cos^2(qd)]+\frac{2q^3}{\varkappa^3}\sin(2qd),$$
$$U_3(q)=\frac{2q}{\varkappa}\sin^2(qd)+\frac{3q^2}{\varkappa^2}\sin(2qd)+\frac{4q^3}{\varkappa^3}\cos^2(qd).$$

The largest increase in T_c is anticipated for the strong defect condition $|\varkappa|\gg k_F$; in what follows we restrict ourselves to $\varkappa\gg k_F$ because addressing the $-\varkappa\gg k_F$ case lies outside the scope of the mean field theory.[3] If $|z|<d/2$ holds then for $\varkappa\gg k_F$ the local density of states becomes

$$N(z)=\frac{m}{\pi^2}\int_0^{k_F}\frac{dq}{(k_F^2-q^2)^{1/2}}\frac{2q^2}{\varkappa^2}\frac{1-\cos(2qz)\cos(qd')}{\sin^2(qd')+4q^4/\varkappa^4}, \quad (7)$$

It is seen that the integrand in (7) is localized near the points

$$q_n=\pi n/d', \quad d'=d+2/\varkappa \quad (8)$$

and may be approximated by a series of δ-function spikes; a similar situation exists for $|z|>d/2$. As a result

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

where $N_0=m/2\pi$, $M=[k_Fd'/\pi]$, and J_0 is the Bessel function. Eq. (9b) implies that the integral over $|z|>d/2$ in (1) is independent of d and so may be performed for the case $d=0$ in which the two defects merge into one; the integral over $|z|<d/2$ yields the oscillatory part of T_c,

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

Substituting (9a) into (1) gives

$$\frac{(\delta T_c)_{\rm osc}}{T_{c0}}=\frac{1}{\pi\lambda_0}\frac{d'}{L}(-2S_1+\frac{4}{\pi}S_1^2+\frac{2}{\pi}S_2), \quad (11)$$
$$S_1=\sum_{n=1}^{[\alpha]}\frac{1}{(\alpha^2-n^2)^{1/2}}, \quad S_2=\sum_{n=1}^{[\alpha]}\frac{1}{\alpha^2-n^2}, \quad \alpha=\frac{k_Fd'}{\pi}.$$

where [...] denotes the integral part of the number. For small values of α the sums S_1 and S_2 contain only a few terms and may be performed directly; in particular, $(\delta T_c)_{\rm osc}=0$ for $0<\alpha<1$. For $\alpha\gg 1$, we can express $(\delta T_c)_{\rm osc}$ in terms of the periodic functions $\psi(\{\alpha\})$ and $f(\alpha)$ (see Fig. 3b)

$$\frac{(\delta T_c)_{\rm osc}}{T_{c0}}=\frac{1}{\pi\lambda_0k_FL}[\ln(2\alpha)-\psi(\{\alpha\})$$
$$+2\pi\sqrt{\alpha}f(\alpha)+4f^2(\alpha)-\pi],$$
$$f(\alpha)=\sum_{n=0}^{\infty}\frac{\cos(2\pi n\{\alpha\}-\pi/4)}{\sqrt{n}}, \quad \alpha=\frac{k_Fd'}{\pi}, \quad (12)$$

where $\psi(z)$ is the logarithmic derivative of the gamma function[10] and {...} represents the fractional part of the number. Near the nth singularity, calculation to leading order in n gives

$$\frac{(\delta T_c)_{\rm osc}}{T_{c0}}\bigg|_{\alpha\to n}=\frac{1}{\pi\lambda_0k_FL}\left[2\pi f_{min}\sqrt{n}+\pi\sqrt{2n}\frac{\theta(\alpha-n)}{\sqrt{\alpha-n}}\right.$$
$$\left.+3\frac{\theta(\alpha-n)}{\alpha-n}\right], \quad (13)$$

where $f_{\rm min}\approx 1.03$ is the minimum value of $f(\alpha)$; the first term in the brackets determining the envelope of the oscillatory minima (Fig. 3a).

The quantity $\delta T_c(0)$ in (10) is calculated by substituting (9b) into (1), which makes the integral of $(\delta N)^2$ logarithmically divergent at large $|z|$. In a dirty superconductor this divergence is cut off at the mean free path l; its finite value is accounted for by replacing

$$\delta(\varepsilon - E_n) \to \frac{1}{\pi} \frac{\gamma}{(\varepsilon - E_n)^2 + \gamma^2} \qquad (14)$$

in (4), so that

$$\delta N(z) \to \delta N(z)\exp(-2|z|/l), \qquad l = v_F/\gamma , \qquad (15)$$

and performing the integral in (1) yields[4)]

$$\frac{\delta T_c(0)}{T_{c0}} = \frac{1}{\pi\lambda_0 k_F L} [\ln(4k_F l) - \pi] . \qquad (16)$$

For a pure superconductor, a logarithmically accurate expression for $\delta T_c(0)$ is obtained by replacing l by L in Eq. (16).

3. T_c OSCILLATIONS WITH CUT-OFF SINGULARITIES

Let us consider the major cutoff mechanisms controlling the singularities involved.

(a) Finite $\varkappa$

For $\varkappa$ finite, the quantity $N(z)$ in the range $|z| < d/2$ takes the form

$$N(z) = \sum_{n=1}^{\infty} A_n[1 - (-1)^n\cos(2q_n z)] , \qquad (17)$$

where

$$A_n = \frac{m}{\pi^2} \int_{-q_n}^{k_F - q_n} \frac{dq}{[k_F^2 - (q_n + q)^2]^{1/2}} \frac{2q_n^2/\varkappa^2}{(qd')^2 + 4q_n^4/\varkappa^4} . \qquad (18)$$

The singularities are due to the Mth term in the sum (17), such that $q_M \approx k_F$; separating this term and assuming $\varkappa = \infty$ for $n \neq M$, we have for T_c

$$\frac{(\delta T_c)_{\text{osc}}}{T_{c0}}\Big|_{\alpha\to n} = \frac{1}{\pi\lambda_0 k_F L} \Big[2\pi f_{min}\sqrt{n} + \frac{2\pi^3 n}{m} A_M + \frac{6\pi^4 n}{m^2} A_M^2\Big] . \qquad (19)$$

By calculating A_M for finite $\varkappa$ we find

$$\frac{(\delta T_c)_{\text{osc}}}{T_{c0}}\Big|_{\alpha\to n} = \frac{1}{\pi\lambda_0 k_F L} \Big[2\pi f_{min}\sqrt{n} + \pi^{3/2} \frac{\varkappa}{k_F} \sqrt{n} F(u) + \frac{3\pi}{2} \frac{\varkappa^2}{k_F^2} F^2(u)\Big] ,$$

$$u = \frac{\pi}{2} \frac{\varkappa^2}{k_F^2} (\alpha - n) , \qquad (20)$$

where the function $F(u)$ determining the shape of the smoothed singularity is given by (Fig. 3c)

$$F(u) = \frac{1}{\pi} \int_0^{\infty} \frac{dx}{\sqrt{x}} \frac{1}{(u - x)^2 + 1} = \frac{1}{\sqrt{2}} \left[\frac{u + (u^2 + 1)^{1/2}}{u^2 + 1}\right]^{1/2} \qquad (21)$$

The envelope of the maxima is obtained from (20) by replacing $F(u) \to F_{\max} = (3/4)^{3/4} \approx 0.81$.

(b) Quasiparticle damping

The finiteness of the mean free path is taken into account by performing the replacement (14) in Eq. (4). The quantity $N(z)$ is then given by Eq. (17) with

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

and $F(u)$ has the same form as (21). Using (19) we find

$$\frac{(\delta T_c)_{\text{osc}}}{T_{c0}}\Big|_{\alpha\to n} = \frac{1}{\pi\lambda_0 k_F L} \Big[2\pi f_{min}\sqrt{n} + 2\pi \sqrt{\frac{\varepsilon_F}{\gamma}} F(u) + 6 \frac{\varepsilon_F}{\gamma} \frac{1}{n} F^2(u)\Big] ,$$

$$u = \frac{2\varepsilon_F}{\gamma} \frac{\alpha - n}{n} . \qquad (23)$$

The envelope of the maxima is obtained by replacing $F(u)$ by $F_{\max}$ and, curiously enough, shows a marked difference from the n dependence given by Eq. (20).

(c) Finite temperature

Representing $N(z)$ by setting $\varepsilon = \varepsilon_F$ in $N(\varepsilon,z)$, Eq. (4), is only valid if $N(\varepsilon,z)$ varies slowly on the energy scale of order ω_0; recognizing that $N(z)$ appears in (1) due to the sum rule for the superconducting kernel $K(\mathbf{r},\mathbf{r}')$

$$\int K(\mathbf{r}, \mathbf{r}')d\mathbf{r}' = V(\mathbf{r})N(\mathbf{r})\ln \frac{1{,}14\omega_0}{T} , \qquad (24)$$

(see the derivation in Ref. 7), we easily conclude that in the general case we should replace $N(z)$ by the quantity

$$N_{eff}(z) \doteq \lambda_0 T \sum_{\omega} \int d\varepsilon \frac{N(\varepsilon, z)}{\varepsilon^2 + \omega^2} , \qquad (25)$$

where the sum is over the Matsubara frequencies $\omega_s = \pi T(2s + 1)$ such that $|\omega_s| < \omega_0$; we have taken into account that $T \approx T_{c0}$. Expressing $N_{\text{eff}}(z)$ in the form of Eq. (17) we find

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

For $\{\alpha\}/\alpha \gg \omega_0/\varepsilon_F$ we retrieve Eq. (13); reversing this inequality gives, by Eq. (19),

$$\frac{(\delta T_c)_{\text{osc}}}{T_{c0}}\Big|_{\alpha\to n} = \frac{1}{\pi\lambda_0 k_F L} \Big[2\pi f_{min}\sqrt{n} + \frac{\pi\lambda_0}{\sqrt{2}} \sqrt{\frac{\varepsilon_F}{T}} G(u) + \frac{3\lambda_0^2}{4} \frac{\varepsilon_F}{T} \frac{1}{n} G^2(u)\Big] , \qquad (27)$$

$$u = \frac{\varepsilon_F}{T} \frac{\alpha - n}{n}, \qquad G(u) = \int_0^{\infty} \frac{dx}{\sqrt{x}} \frac{\text{th}(x - u)}{x - u} .$$

The singularities are cut off at $\{\alpha\}/\alpha \sim T/\varepsilon_F$; in the range $T/\varepsilon_F \ll \{\alpha\}/\alpha \ll \omega_0/\varepsilon_F$ they have logarithmic corrections and therefore cannot be described by the pure power law form (13). The function $G(u)$ determining the shape of the maxima is shown in Fig. 3c; the envelope of the maxima is obtained from (27) by replacing $G(u) \to G_{\max} \approx 3.8$.

4. DISCUSSION

From Eqs. (20), (23), and (27) it follows that the maximum T_c increase occurs when

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

and its value is

$$\frac{\delta T_c}{T_{c0}} \sim \frac{\varepsilon_F}{T_c}\frac{a}{L}, \tag{29}$$

showing that δT_c becomes $\sim T_{c0}$ for $L \sim \xi_0$; for $\delta T_c \gtrsim T_{c0}$ the initial formula (1) breaks down, but physical arguments suggest a further increase in T_c as L is decreased below ξ_0. The limiting value of (29) may in fact be unattainable because of the effects the instability of the Fermi level near the singularity may have on the system (dielectrization of the spectrum due to structural transitions; antiferromagnetic ordering, symmetry-conserving strains,[11] etc.).

As $\varkappa \to \infty$, the two-dimensional superconductor decomposes into a system of disconnected one-dimensional strips whose superconductivity is destroyed by fluctuations. In one dimension, the condition for the fluctuations to be unimportant is $J_\perp \gtrsim T_c$[12], where $J_\perp$ is the transverse overlap integral; if we set $J_\perp \sim \varepsilon_F (\varkappa a)^{-1}$, the upper bound on $\varkappa$ is (for $d \sim a$)

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

which turns out to be compatible with (28).

The plane defect structure required (Fig. 1) may be produced (a) by controlling the twinning process (which always operates in the direction normal to the Cu–O layers); (b) by introducing atomic layers of a dissimilar material (superconducting oxide superlattices, periodic normal to the c-axis with a period ~ 100 Å, have already been reported[13]); and (c) by depositing thin (a few Cu–O layers) oxide layers onto artificially periodic substrates.

Finally, the T_c enhancement effect also occurs for a random distribution of defects (with average separation L). Suppose the defect separation d fluctuates by the amount δd such that $k_F^{-1} \ll \delta d \ll d, L$; then averaging Eqs. (20), (23), and (27) over d and using Eqs. (10) and (16) we obtain

$$\frac{\delta T_c}{T_{c0}} = \frac{1}{\pi \lambda_0 k_F L} \times \left\{ 3 \ln \left[\max \left(\frac{\varkappa^2}{k_F^2}, \frac{\varepsilon_F}{\gamma k_F d}, \frac{\varepsilon_F}{T k_F d} \right) \right] + \ln [\max(k_F l, k_F L)] + \ln (k_F d) + O(1) \right\},$$

indicating that the estimate $\delta T_c \sim T_{c0}\, a/L$ acquires a large logarithmic factor in this case. Qualitatively, this is also true for the case $\delta d \sim d \sim L$, i.e., for a perfectly random defect distribution. It is perhaps not unlikely that the high concentration of the plane defects or their lucky distribution in space may account for the irreproducible observation of unusually high T_c's in the early high-temperature superconductivity studies.

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1) Because the exact mechanism of high-temperature superconductivity is not yet known, this assumption is, admittedly, somewhat questionable, but in our view no experimental evidence has been found to contradict it.

2) At a qualitative level, our results also hold for $d \sim L$, which is a simpler case experimentally.

3) For $-\varkappa \gg k_F$, mean field theory predicts the Tamm-state-induced localization of the order parameter near the linear defects.[7] Since for $d \gg a$ this localization is destroyed by fluctuations, it follows that, unlike the three-dimensional case, in two dimensions the Tamm states are of no consequence qualitatively and the results for $\varkappa \gg k_F$ should be similar to those for $-\varkappa \gg k_F$.

4) Although performed for a pure superconductor, the derivation of Eq. (1) in Ref. 7 also holds in the dirty limit, provided the superconducting kernel $K(z,z')$ is replaced by $\langle K(z,z') \rangle$, its average over the impurity positions. Accordingly, $N(z)$ in (1) gives way to an averaged quantity $\langle N(z) \rangle$, expressible through the imaginary part of the average Green's function $\langle G(z,z) \rangle$; the damping of quasiparticles is taken into account by replacing $\varepsilon \to \varepsilon + i\gamma$ in $\langle G(z,z) \rangle$, which operation is equivalent to Eq. (14).

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