Mechanism of the superconductivity of twinning planes

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The problem of calculation of T_c of a superconductor with a planar defect is solved subject to fairly general assunptions about the defect. The equivalence of superconducting properties is demonstrated for a topological defect of a twinning plane type and a scattering defect in the form of a monolayer of foreign atoms. A system of nonlinear equations for a localized superconductivity is derived. It is shown that in addition to a phenomenological Buzdin–Bulaevskiĭ picture [Sov. Phys. JETP **57**, 426 (1983)], it is possible to provide a different explanation which alters radically the interpretation of the experimental results of Khaĭkin and Khlyustikov [JETP Lett. **33**, 158 (1981); **36**, 164 (1982); **38**, 224 (1983); Adv. Phys. **36**, 271 (1987)] and, in contrast to the former, can give reasonable values of microscopic parameters. Systems of periodically distributed planar defects are investigated. An analysis is made of the possibility of reaching high values of T_c in a system of this kind because of Van Hove singularities in the spectrum of two-dimensional Tamm energy bands.

1. INTRODUCTION

Khaĭkin and Klyustikov[1] discovered a localized superconductivity near twinning boundaries in Sn at a temperature $\delta T_c = 0.04$ K higher than the transition at $T_{c0} \approx 3.7$ K in bulk tin. This effect can be described phenomenologically on the assumption that in a layer of thickness of the order of the interatomic distance a near a boundary the electron–phonon interaction constant λ increases by an amount $\delta\lambda$ compared with its bulk value λ_0 (Ref. 2). Assuming that $T_c = T_{c0} + \delta T_c$ is governed by the value of λ averaged on a scale of $\xi(T_c) \sim \xi_0 (T_{c0}/\delta T_c)^{1/2}$ (ξ_0 is the coherence length), we readily obtain[2]

$$\frac{\delta T_c}{T_{c0}} \sim \left(\frac{\delta\lambda}{\lambda_0^2}\frac{a}{\xi_0}\right)^2. \quad (1)$$

Substituting the values $\delta T_c / T_{c0} \sim 10^{-2}$, $a/\xi_0 \sim 10^{-3}$, and $\lambda_0 \approx 0.3$ for tin, we find that the change in λ is very large: $\delta\lambda/\lambda_0 \sim 30$. This conclusion is supported partly by the experimental results: in small particles containing twinning planes the suppression of the proximity effects makes it possible to raise T_c to 12 K (Ref. 1).

The following obvious questions should be asked: is indeed the increase in λ so large, what is the mechanism of this increase, and whether this mechanism can be used in developing high-temperature superconductors? These questions not answered in published papers. The mechanisms proposed in Refs. 3 and 4 and based on a change in the phonon properties near a twinning boundary predict an effect which is far too small. The possibility of initiation of a localized superconductivity because of a superconducting transition in a two-dimensional Tamm energy band is considered in Ref. 5. For certain relationships between the parameters of a postulated two-band model the value of T_c is close to the temperature of the transition of two-dimensional electrons which is in no way related to T_{c0}. However, in view of the phenomenological nature of the parameters used, it is not clear whether this situation is realistic from the microscopic point of view. Moreover, the very model used in Ref. 5 can be objected to: in the presence of a split-off two-dimensional energy band the wave functions of three-dimensional electrons cannot be plane waves in view of analytic properties of the amplitude of the scattering by a planar defect. We shall demonstrate however that under certain conditions the results of Ref. 5 can be given a microscopic explanation. It is shown in Ref. 6 that $\delta T_c \sim T_{c0}$ because of a change in the states in a continuous spectrum without allowance for the contribution Tamm levels;, we shall show that this result is incorrect.

We shall attempt a consistent microscopic analysis developing the ideas put forward earlier by the present authors[7] and based on an investigation of the BCS Hamiltonian generalized to the case of a spatial inhomogeneity[8]:

$$\hat{H} = \int d\mathbf{r} \Big\{ \hat{\Psi}_\alpha^+(\mathbf{r}) \hat{H}_0 \hat{\Psi}_\alpha(\mathbf{r}) - \frac{1}{2} V(\mathbf{r}) \hat{\Psi}_\alpha^+(\mathbf{r}) \hat{\Psi}_\beta^+(\mathbf{r}) \hat{\Psi}_\beta(\mathbf{r}) \hat{\Psi}_\alpha(\mathbf{r}) \Big\}, \quad (2)$$

$$\hat{H}_0 = \mathbf{p}^2/2m + U(\mathbf{r}),$$

where $U(\mathbf{r})$ is the potential of a lattice with a twin boundary and $V(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$ is the potential of the electron–electron interaction.

2. QUALITATIVE PICTURE

A twinning plane (Fig. 1a) differs from a monolayer of foreign atoms (Fig. 1b) by the following topological property: for a fixed selection of the coordinate (reference) system the electron spectra $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$ to the right and left are different, although they are related by a symmetry transformation. It is interesting to consider the following question: are the topological properties of a twinning plane important in the case of the effects reported in Ref. 1? According to the Hamiltonian of Eq. (2), the answer must be negative; in particular, if the actual wave functions of an electron vary sufficiently slowly, a rigorous theorem (Sec. 4) applies: for each twinning plane we can identify a defect of the type shown in Fig. lb (we shall call it a scattering defect), which has identical superconducting properties. In the present section we shall consider the simpler case of a scattering defect

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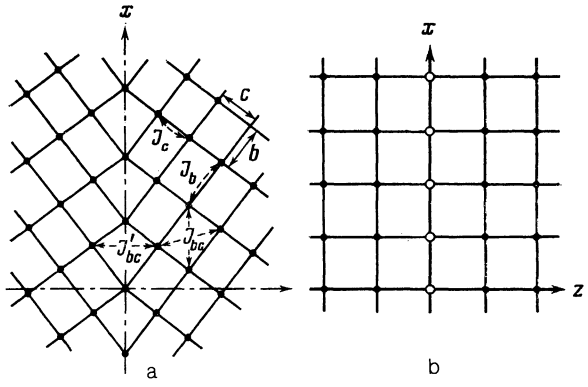

FIG. 1.

assumed to be lying in the $z = 0$ plane.

In view of the translational invariance in the xy plane the one-electron wave functions are

$$\Psi_n(\mathbf{r}) = S^{-1/2}\exp(ik_\parallel r_\parallel)\varphi_{sk_\parallel}(z), \quad r_\parallel = (x, y), \quad k_\parallel = (k_x, k_y), \tag{3}$$

(s is the transverse quantum number and S is the area of the system in the xy plane), where the functions $\varphi_{sk_\parallel}(z)$ satisfy a one-dimensional Schrödinger equation describing a chain with a defect at the origin of the coordinate system. The spectrum of this equation represents a set of bands with a local level split off from each of them; if we allow for the longitudinal quasimomentum $k_\parallel$, we find that local levels become two-dimensional energy bands and the complete spectrum assumes the form shown in Fig. 2. Splitting of two-dimensional bands is the main effect that gives rise to a localized superconductivity.

A natural generalization of the constant $\lambda = VN(0)$ to the inhomogeneous case is a function

$$\lambda(\mathbf{r}) = V(\mathbf{r})N(0, \mathbf{r}), \tag{4}$$

where $N(\varepsilon)$ and $N(\varepsilon, \mathbf{r})$ are the average and local densities of states:

$$N(\varepsilon) = \Omega^{-1}\sum_n \delta(\varepsilon - \varepsilon_n), \tag{5}$$

$$N(\varepsilon, \mathbf{r}) = \sum_n |\Psi_n(\mathbf{r})|^2\delta(\varepsilon - \varepsilon_n) = \frac{1}{S}\sum_{k_\parallel}\sum_s \delta(\varepsilon - \varepsilon_s(k_\parallel))\,|\varphi_{sk_\parallel}(z)|^2 \tag{6}$$

(energies are measured from the Fermi level and Ω is the volume of the system). It follows from Eq. (3) that $N(\varepsilon, \mathbf{r})$ depends only on z and can be represented in the form

$$N(\varepsilon, z) = N_0(\varepsilon) + N_{loc}(\varepsilon, z) + N_c(\varepsilon, z), \tag{7}$$

so that for $V(\mathbf{r}) = \text{const}$ we can introduce splitting of $\lambda(z)$:

$$\lambda(z) = \lambda_0 + \lambda_{loc}(z) + \lambda_c(z) \equiv \lambda_0 + \delta\lambda(z). \tag{8}$$

Here, $N_0(\varepsilon)$ is the density of states in an ideal crystal, $N_c(\varepsilon, z)$ is the effect of changes in the states in the continuous spectrum in the sum of Eq. (6) for s, and $N_{\text{loc}}(\varepsilon, z)$ is associated with local levels: in the case of one level this is simply the zeroth term of the sum over s in Eq. (6):

$$N_{loc}(\varepsilon, z) = \frac{|\varphi_0(z)|^2}{S}\sum_{k_\parallel}\delta(\varepsilon - \varepsilon_0(k_\parallel)) = N_{2D}(\varepsilon)\,|\varphi_0(z)|^2, \tag{9}$$

where $\varepsilon_0(k_\parallel)$ and $N_{2D}(\varepsilon)$ are the spectrum and the density of states of a split-off two-dimensional band [we are ignoring the dependence of $\varphi_0(z)$ on $k_\parallel$]. The quantity $N_{\text{loc}}(\varepsilon, z)$ is positive and it increases locally λ, but it can be compensated by $N_c(\varepsilon, z)$ (Fig. 3).

A two-dimensional band of finite width must have Van Hove singularities $N_{2D}(\varepsilon) \propto \ln|\varepsilon - \varepsilon_0|$, which can increase strongly $N_{\text{loc}}(\varepsilon, z)$. Bearing in mind that in the calculation of T_c the singularities are truncated on the scale of the Debye energy ω_D (see the Appendix 1), we obtain an estimate for the maximum value of $\delta\lambda$:

$$(\delta\lambda)_{\max}/\lambda_0 \sim m\ln(J/\omega_D), \tag{10}$$

where J is the bandwidth and m is the number of the Van Hove singularities which can be large (in the case of Sn the Fermi level intersects five three-dimensional bands and, consequently, four two-dimensional bands and each of them several Van Hove singularities). Inclusion of $N_c(\varepsilon, z)$ does not alter the estimate given by Eq. (10), because $N_c(\varepsilon, z) \leqslant N_0(\varepsilon)$. In principle, the ratio $\delta\lambda/\lambda_0$ can be large, but it is unlikely to be ~ 30.

The difficulty outlined above can be solved as follows. The estimate given by Eq. (1) is based on the assumption that the superconducting order parameter $\Delta(z)$ varies slowly near a defect, so that $\delta\lambda$ is averaged on the scale of $\xi(T)$. However, if $\Delta(z)$ has a sharp peak near $z = 0$, then the vicinity of the defect is characterized by a large weight in the averaging procedure and T_c is higher than predicted by Eq. (1). An analysis shows that $\Delta(z)$ can be represented in the form[1)]

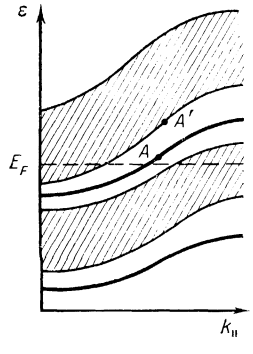

FIG. 2.

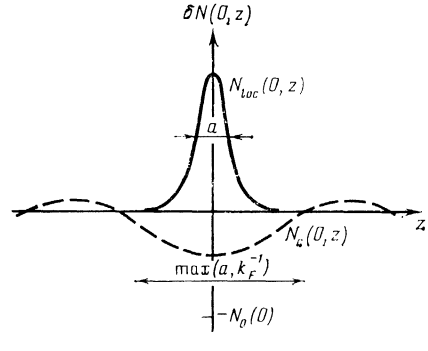

FIG. 3.

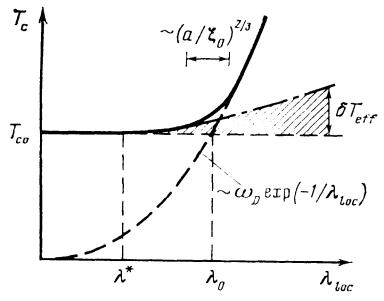

FIG. 4. Dependence of the transition temperature T_c on the parameter λ_{loc} representing the amplitude $\lambda_{\text{loc}}(z)$; Here λ^* is the lower limit of existence of a localized superconductivity. The shaded region identifies the conditions under which it should be possible to observe a localized superconductivity in practice.

$$\Delta(z)=\Delta_0(z)+\psi(z), \tag{11}$$

where the function $\Delta_0(z)$ is localized at $|z| \lesssim a$ and $\psi(z)$ varies on the scale of $\xi(T)$. If $\lambda_{\text{loc}} \lesssim \lambda_0$ [λ_{loc} represents the amplitude of $\lambda_{\text{loc}}(z)$] the amplitude of the peak is small, $\Delta_0(z) \lesssim \psi(0)$, and T_c can be estimated on the basis of Eq. (1); however, if $\lambda_{\text{loc}} \gtrsim \lambda_0$, it is found that $\Delta_0(z) \sim \psi(0)\xi_0/a$, i.e., the order parameter is localized at an atomic distance from a defect and it has only small "tails" extending to distances $\sim\xi(T)$; we then find that $\delta T_c \sim T_{c0}$ (Fig. 4). It is interesting that the strongly localized regime appears only when the increase in λ is associated with $N(0,\mathbf{r})$; however, if it is related to $V(\mathbf{r})$ and we have $N(0,\mathbf{r}) = \text{const}$, then the estimate given by Eq. (1) is valid right up to $\delta\lambda/\lambda_0 \sim \xi_0/a$,, i.e., practically always.

According to the theory of Ref. 2, a localized superconductivity can exist if the following quantity is positive:

$$a\delta\lambda \equiv \int \delta\lambda(z)\,dz = \int [\lambda_{\text{loc}}(z) + \lambda_c(z)]\,dz, \tag{12}$$

which for $V(\mathbf{r}) = \text{const}$ is governed by the change in the average density of states $N(0)$ and is equally likely to have either sign; for example, it may be positive if a Van Hove singularity A (Fig. 2) is closer to the Fermi level as a result of splitting of the two-dimensional band than in the unsplit state A', but it can be negative in the opposite case. Experiments however indicate a shift of the probability in the direction of a localized superconductivity: it was found in five metals and reported in seven papers.[1] According to the proposed theory, the quantity (12) must be positive only in the case of a weakly scattering defect when the radius of a bound state a is large and the amplitudes $N_c(\varepsilon,z)$ and $N_{\text{loc}}(\varepsilon,z)$ are small (Fig. 3). In the case of a sufficiently strong defect because of the smallness of a, we find that the condition $\lambda_{\text{loc}} \gtrsim \lambda_0$ is satisfied [$N_{2D}(\varepsilon)$ in Eq. (9) is limited from below by a value of the atomic order] and a localized superconductivity can exist irrespective of the value of $\lambda_c(z)$: the point λ^* in Fig. 5 depends on $\lambda_c(z)$, but it is always smaller than λ_0.

If $\lambda_{\text{loc}} \gtrsim \lambda_0$, the function $\Delta(z)$ is localized at $|z| \lesssim a$ and T_c is so low that it is practically undetectable (the sensitivity of the magnetometer used in the investigation reported in Ref. 1 made it possible to detect an ideal diamagnetic layer of thickness $\gtrsim 10a$). A localized superconductivity can be observed only in the vicinity of T_{c0}: $T_{c0} < T \lesssim T_{c0} + \delta T_{\text{eff}}$,

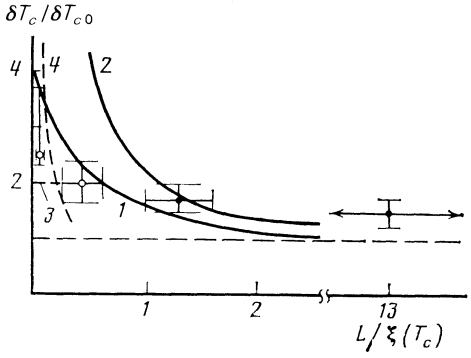

FIG. 5. Dependence of the temperature range of existence of a localized superconductivity δT_c on the distance L_0 between twinning planes (δT_{c0} is the value for a single twinning plane): ●) experimental points for two closely spaced planes; ○) sample with a high density of twinning planes. According to Ref. 2, the black dots should lie on curve *1* and the open circles on curve *2*. According to the theory proposed in the present paper, the range δT_c is δT_{eff} and the adopted analysis of the experimental results is meaningful only if $L_0 \ll \xi(T_c)$ (Sec. 7); then, the black dots reach the value 2 (curve *3*) and the open circles fit the dependence $L_0^{-2/3}$ with an undetermined coefficient, as represented by curve *4* (the coefficient is selected to ensure the best agreement with the experimental results).

when the amplitude $\psi(z)$ becomes sufficiently large; if $\lambda_{\text{loc}} \gg \lambda_0$ (Sec. 6), then

$$\frac{\delta T_{\text{eff}}}{T_{c0}} \sim \frac{T_c}{T_{c0}} \frac{a}{\xi_0}. \tag{13}$$

Substituting $\delta T_{\text{eff}}/T_{c0} \sim 10^{-2}$, and $a/\xi_0 \sim 10^{-3}$, we obtain $T_c/T_{c0} \sim 10$, which corresponds to $\delta\lambda/\lambda_0 \sim 3$.

In the case of two closely spaced twinning planes the quantity a is replaced with $2a$ and the temperature range of existence of a localized superconductivity widens fourfold according to Eq. (1) and twofold according to Eq. (13). For a system of twinning planes distributed periodically at a distance $L_0 \ll \xi(T_c)$, we find that $\delta T_c \propto L_0^{-1}$, and, according to Ref. 2, $\delta T_{\text{eff}} \propto L_0^{-2/3}$ follows from Sec. 7; the true value of T_c for $\lambda_{\text{loc}} \gtrsim \lambda_0$ is practically independent of L_0: a reduction in L_0 simply improves the conditions for its observation (the critical current, magnetic moment, etc. increase). Therefore, if $\lambda_{\text{loc}} \gtrsim \lambda_0$, the predictions of the proposed theory differ from the predictions given in Ref. 2 even at the phenomenological level, which can be used as an experimental check (Fig. 5).

It follows from the above discussion that in the case of twinning boundaries in Sn the ratio $\delta\lambda/\lambda_0$ amounts to a few units, whereas according to Eq. (10) it can be considerably larger. Therefore, we should seek defects characterized by a higher value of $\delta\lambda/\lambda_0$. For example, it is possible to introduce monolayers of a foreign material into a superconductor and alter this monolayer so as to control the positions of the Van Hove singularities. Modern apparatus can be used to create such structures; then, in contrast to the systems with twins considered above, the concentration of planar defects can be very high. We cannot exclude the possibility that the high-temperature superconductivity of oxides[9] could also be interpreted by the proposed scheme if the Cu–O planes are considered as planar defects; in particular, a quasiphase transition at $\lambda_{\text{loc}} \approx \lambda_0$ (Fig. 4) can be used to interpret the "superconducting explosion" of 1987 (Ref. 7).

3. INITIAL EQUATIONS

We shall now postulate the properties of planar defects which we shall use later (Secs. 5–7); they will be justified in Sec. 4 on the basis of certain model representations.

1. We shall assume a translational invariance in the xy plane so that the wave functions can be written in the form of Eq. (3); we shall ignore the difference between the Bloch functions of an ideal crystal and plane waves.

The equations for the superconductivity of a system described by the Hamiltonian of Eq. (2) are the usual Gor'kov equations,[10] but the Matsubara Green function $G_\omega(\mathbf{r},\mathbf{r}')$ for a normal metal, which occurs in the above equations, should be deduced from the eigenfunctions of the Hamiltonian $\hat{H}_0$; in view of separation of the variables, we find that

$$G_\omega(\mathbf{r},\mathbf{r}')=\frac{1}{S}\sum_{k_\parallel}\exp[ik_\parallel(r_\parallel-r_\parallel')]G_{\omega k_\parallel}(z,z'), \tag{14}$$

$$G_{\omega k_\parallel}(z,z')=\sum_s\frac{\varphi_{sk_\parallel}(z)\varphi^*_{sk_\parallel}(z')}{i\omega-\varepsilon_s(k_\parallel)}.$$

Iteration of the Gor'kov equation can yield an equation containing only the superconducting gap $\Delta(\mathbf{r})$ as the unknown function (Ref. 11); if we allow for the one-dimensional nature of the geometry of the problem, we find that the corresponding result is

$$\begin{aligned}\Delta(z)=V(z)T\sum_{|\omega|<\omega_D}\int\frac{d^2k_\parallel}{(2\pi)^2}\Big\{&\int dz_1\,G_{\omega k_\parallel}(z,z_1)\\&\times\Delta(z_1)G_{-\omega k_\parallel}(z_1,z)\\&-\int dz_1\,dz_2\,dz_3\,G_{\omega k_\parallel}(z,z_1)\Delta(z_1)G_{-\omega k_\parallel}(z_1,z_2)\\&\times\Delta^*(z_2)G_{\omega k_\parallel}(z_2,z_3)\Delta(z_3)\\&\times G_{-\omega k_\parallel}(z_3,z)+\ldots\Big\}\end{aligned} \tag{15}$$

[nth term of the series on the right-hand side contains $2n$ functions $G_{\omega k_\parallel}$ and $2n-1$ functions $\Delta(z)$ with the common coefficient $(-1)^{n+1}$].

2. We shall assume the presence of a split-off two-dimensional band, so that one of the function $\varphi_s(z)$, for example that characterized by $s=0$, is localized at $|z|\lesssim a$. Separating the zeroth term in the sum over s in Eq. (14), we obtain the splitting

$$\begin{aligned}&G_{\omega k_\parallel}(z,z')=\tilde{G}_{\omega k_\parallel}(z,z')+G^{loc}_{\omega k_\parallel}(z,z'),\\&G^{loc}_{\omega k_\parallel}(z,z')=\frac{\varphi_0(z)\varphi_0^*(z')}{i\omega-\varepsilon_0(k_\parallel)}.\end{aligned} \tag{16}$$

We shall ignore the dependence of $\varphi_0(z)$ on $k_\parallel$ which is rigorously justified for the spectrum $\varepsilon(\mathbf{k})=\varepsilon_1(k_\parallel)+\varepsilon_2(k_z)$.

3. The function $\tilde{G}_{\omega k_\parallel}(z,z')$ is of the order of $1/v_F$ and it is localized because of the difference between the arguments on the scale of $v_F/\omega\sim\xi_0$, whereas for $z,z'\gtrsim\xi_0$ and $-z,-z'\gtrsim\xi_0$ it is identical with the Green functions $G^{(1)}_{\omega k_\parallel}(z-z')$ and $G^{(2)}_{\omega k_\parallel}(z-z')$ for the right- and left-hand halves of a crystal.

4. We shall assume that the right- and left-hand halves of a crystal are identical or are related by mirror symmetry so that the functions $G^{(1)}_{\omega k_\parallel}(z-z')$ and $G^{(2)}_{\omega k_\parallel}(z-z')$ are linked by one of the following relationships:

$$G^{(1)}_{\omega k_\parallel}(z-z')=G^{(2)}_{\omega k_\parallel}(z-z'),\quad G^{(1)}_{\omega k_\parallel}(z-z')=G^{(2)}_{\omega k_\parallel}(z'-z). \tag{17}$$

The kernel $K(z,z')$ of a linearized equation (15),

$$\Delta(z)=\int dz'\,K(z,z')\Delta(z'), \tag{18}$$

has the same value $K_0(z-z')$ for $z,z'\gtrsim\xi_0$ and $-z,-z\gtrsim\xi_0$ because of Eq. (17) and in this case we have the splitting which follows from Eq. (16) and if we ignore the convolutions $\tilde{G}G^{loc}$, which are small on the scale of $\sim a/\xi_0$ (see Sec. 6), we find that

$$K(z,z')=K_0(z-z')+K_c(z,z')+K_{loc}(z,z'), \tag{19}$$

$$K_{loc}(z,z')=V(z)T\sum_\omega\int\frac{d^2k_\parallel}{(2\pi)^2}\frac{|\varphi_0(z)|^2|\varphi_0(z')|^2}{\varepsilon_0(k_\parallel)^2+\omega^2}, \tag{20}$$

where $K_0(z-z')$ is localized at $|z-z'|\lesssim\xi_0$, $K_c(z,z')$ at $|z|$, $|z'|\lesssim\xi_0$, and $K_{loc}(z,z')$ at $|z|,|z'|\lesssim a$.

5. It follows from Eq. (19) and from the sum rule for the kernel $K(z,z')$ that[8]

$$\int K(z,z')\,dz'=\lambda(z)\ln\frac{1.14\omega_D}{T}, \tag{21}$$

yields the splitting (8) for $\lambda(z)$ and the function $\lambda_c(z)$ is localized near $z=0$ not on the scale of ξ_0, but at an atomic distance because of the specific alternating-sign structure of the kernel $K_c(z,z')$.

4. ELECTRONIC PROPERTIES OF PLANAR DEFECTS

We shall now justify the properties of planar defects postulated in Sec. 3. The eigenfunctions of the Hamiltonian $\hat{H}_0$ will be sought in the site representation considering, for the sake of simplicity, just one energy band:

$$\sum_{\mathbf{r}'}J(\mathbf{r},\mathbf{r}')\Psi(\mathbf{r}')=E\Psi(\mathbf{r}). \tag{22}$$

In the case of defects shown in Fig. 1 a translational invariance in the xy plane is self-evident and it means that $J(\mathbf{r},\mathbf{r}')=J(r_\parallel'-r_\parallel;z,z')$. Separating in Eq. (22) the longitudinal motion, we obtain

$$\begin{aligned}&\sum_{z'}J_{zz'}(k_\parallel)\varphi(z')=E\varphi(z),\\&J_{zz'}(k_\parallel)=\sum_{r_\parallel}J(r_\parallel;z,z')\exp(ik_\parallel r_\parallel).\end{aligned} \tag{23}$$

Scattering defect. For a scattering defect (Fig. 1b) and a fixed value of $k_\parallel$ the overlap integrals $J_{zz'}$ have the property

$$J_{zz'}=J^{(0)}_{z'-z}+\delta J_{zz'}, \tag{24}$$

where $\delta J_{zz'}$ is localized in $|z|,|z'|\lesssim a$.

1. The problem of existence of a local level can be solved by the Lifshitz method.[12] Introducing the Green function of an ideal crystal $G^0_E(z-z')$ and applying Eq. (24), we can write down Eq. (23) in an integral form. The limits of the spectrum $\varepsilon(k_\parallel,k_z)$ for an ideal crystal with a fixed value of $k_\parallel$ will be assumed to correspond to quasimomenta $k_z=k_0$ and $k_z=k_1$; if $E\approx\varepsilon(k_\parallel,k_\alpha)$, and $\alpha=0$ or 1, we have

$$\begin{aligned}&G_E{}^0(z-z')=\bar{G}_E(z-z')\exp[ik_\alpha(z-z')],\\&\varphi(z)=\bar{\varphi}(z)\exp(ik_\alpha z),\end{aligned} \tag{25}$$

where $\overline{G}_E(z)$ and $\overline{\varphi}(z)$ are slowly varying functions of z. Then Eq. (23) yields

$$\bar{\varphi}(z)=\bar{\varphi}(0)\overline{G}_E(z)W_\alpha,$$
$$W_\alpha=\sum_{z,z'}\delta J_{zz'}\exp[ik_\alpha(z'-z)]. \tag{26}$$

Assuming that $z=0$, we obtain the following equation for a local level[12]: in view of the divergence $\overline{G}_E(0)=G_E^{(0)}(0)$ in the limit $E\to\varepsilon(k_\parallel,k_\alpha)$, it can exist even for infinitesimally small values of $\delta J_{zz'}$. In the case of a diagonal defect we have $\delta J_{zz'}=\delta J_z\delta_{zz'}$, the equality $W_0=W_1$ is valid, and the level exists always; if $W_0>0$, it splits from the upper edge of the energy band, whereas for $W_0<0$ it splits off from the lower edge. In the case of the nondiagonal defect we have $W_0\neq W_1$ and the situation becomes more complex: if $W_0,W_1>0$ the level splits upward, whereas for $W_0,W_1<0$ it splits downward, for $W_0>0$, $W_1<0$ it is absent, and for $W_0<0$, $W_1>0$ there are levels split off from both edges of the energy band. In the case of typical metals this complication is unimportant: the Fermi level intersects several energy bands (Fig. 2) and on the average one levels splits off from each band.

2. Near the band edge any defect appears to be pointlike so that $\delta_{zz'}=W\delta_{z0}\delta_{z'0}$, and for such a defect we can readily find the Green function for Eq. (23):

$$G_E(z,z')=G_E^0(z-z')+G_E^0(z)W[1-WG_E^0(0)]^{-1}G_E^0(-z'). \tag{27}$$

The required function $G_{\omega k_\parallel}(z,z')$ is then obtained by the substitution $E\to i\omega$. We shall assume that near the band edge we have

$$\varepsilon(k_\parallel,k_z)=\sum_z J_z^{(0)}(k_\parallel)e^{ik_zz}=-\varepsilon_F+\frac{k_\parallel^2}{2m_\parallel}+\frac{k_z^2}{2m},$$
$$k_z^0=[2m(\varepsilon_F-k_\parallel^2/2m_\parallel)]^{1/2},\ v_z=k_z^0/m,\ \varkappa=-mW \tag{28}$$

(ε_F is the Fermi level measured from the band edge). Equation (27) depends on a parameter $(k_z^0)^2=2m(\varepsilon_F-k_\parallel^2/2m_\parallel)$, and integration with respect to $k_\parallel$ in Eq. (15) covers the range $(k_z^0)^2>0$, and also $(k_z^0)^2<0$, where we have correspondingly

$$G^0_{\omega k_\parallel}(z)\propto\exp(-|\omega z|/v_z),\quad G^0_{\omega k_\parallel}(z)\propto\exp(-|k_z^0|\,|z|).$$

In the second range of existence the important region is that in the vicinity of a pole $(k_z^0)^2=-\varkappa^2$, where $G_{\omega k_\parallel}$ is identical with the function $G^{\rm loc}_{\omega k_\parallel}$, defined by Eq. (16). The function $\tilde{G}_{\omega k_\parallel}$ which results from the splitting of Eq. (16) is relatively small, $\sim 1/v_F$, in the main range of the values of $k_\parallel$ and it plays an important role in Eq. (15) only if its radius of localization in respect of z and z' is large, i.e., in the range $\varepsilon_F-k_\parallel^2/2m_\parallel\sim\varepsilon_F$:

$$\tilde{G}_{\omega k_\parallel}(z,z')=G^0_{\omega k_\parallel}(z,z')+G^c_{\omega k_\parallel}(z,z'),$$
$$G^0_{\omega k_\parallel}(z-z')=-\frac{i\,\mathrm{sgn}\,\omega}{v_z}\exp(ik_z^0|z-z'|\,\mathrm{sgn}\,\omega)\times\exp\left(-\frac{|\omega|\,|z-z'|}{v_z}\right), \tag{29}$$
$$G^c_{\omega k_\parallel}(z,z')=\frac{1}{v_z}\frac{\varkappa}{k_z^0-i\varkappa\,\mathrm{sgn}\,\omega}\exp[ik_z^0(|z|+|z'|)\,\mathrm{sgn}\,\omega]\times\exp\left[-\frac{|\omega|(|z|+|z'|)}{v_z}\right].$$

The properties Sec. 3 are given by the system of equations (29).

3. The local density of states $N(0,z)$ can be found from

$$N(0,z)=-\lim_{\omega\to0}\frac{\mathrm{sgn}\,\omega}{\pi}\,\mathrm{Im}\int\frac{d^2k_\parallel}{(2\pi)^2}G_{\omega k_\parallel}(z,z). \tag{30}$$

If we represent $N(0,z)$ in the form of Eq. (7), we find that the asymptote $N_c(0,z)$ is described by

$$N_c(0,z)=\begin{cases}-\dfrac{m_\parallel}{2\pi}\varkappa\theta(\varkappa)e^{-2\varkappa|z|}, & k_F\gg\varkappa\\ -\dfrac{m_\parallel}{4\pi^2}\dfrac{\sin 2k_Fz}{z}, & k_F\ll\varkappa\end{cases}, \tag{31}$$

where $k_F=(2m\varepsilon_F)^{1/2}$. Hence, it is obvious that $\lambda_c(z)$ is localized at $|z|\lesssim a$.

4. In a system of finite length L along the z axis we find that Eq. (31) remains valid to within $\sim a/L$ inclusive, so that the contribution of a defect to the average density of states $N(\varepsilon)$ of Eq. (5), which is of the order of a/L, appears only in the vicinity of the defect and can be found by integration of Eq. (31) with respect to z [in calculations accurate to within $\sim a/L$ the quantities $N(\varepsilon)$ and $N(\varepsilon,z)$ should be understood to be the functions which are smoothed out in order to eliminate the size quantization effects[13]].

At first sight the change in $N(\varepsilon)$ should result in a small ($\sim a/L$) shift of the Fermi level, in accordance with the relationship

$$\int_{-\infty}^{\varepsilon_F}N_0(\varepsilon)\,d\varepsilon=\int_{-\infty}^{\varepsilon_F+\delta\varepsilon_F}N(\varepsilon)\,d\varepsilon, \tag{32}$$

which should be allowed for in a discussion of periodic structures in Sec. 7. However, the change in $N(\varepsilon)$ is acquired only in the vicinity of a defect $|z|\lesssim a$, so that a shift of the Fermi level causes charge separation; a charge surface density $\sim e/a^2$ appears in a defect, whereas a compensating bulk density $\sim e/a^2L$ is formed in the bulk. Consequently, an electric field $\mathscr{E}\sim e/a^2$ appears in a sample and its energy is $\sim e^2L/a^2$ per unit cell of the surface. This energy can be reduced to $\sim e^2/a$ by: a) a redistribution of electrons resulting in screening of the excess defect charge on a scale of $\sim a$; b) creation, near a defect, of a lattice deformation which compensates the excess electron charge because of a change in the ion concentration. The effects a) and b) suppress the shift of the Fermi level by altering the scattering properties of a defect, which should now be determined in a self-consistent manner. Under equilibrium conditions we have a relationship similar to the Friedel sum rule[14]:

$$\int_{-\infty}^{\varepsilon_F}d\varepsilon\int_{-\infty}^{\infty}dz[N_{loc}(\varepsilon,z)+N_c(\varepsilon.z)]=Z_{eff}. \tag{33}$$

where $|e|Z_{\rm eff}S$ is the excess charge of the ions localized near a defect. In the case of a point defect the relationship (33) links $\varkappa$ to $Z_{\rm eff}$.

Twinning plane. In the simplest case a twinning plane is

a plane of mirror symmetry and the overlap integrals of Eq. (23) have the property ($J_z^{(0)} \neq J_{-z}^{(0)}$)

$$J_{zz'}=J_{z'-z}^{(0)} \text{ for } z,z' \gg a, \quad J_{zz'}=J_{z-z'}^{(0)} \text{ for } -z,-z' \gg a. \quad (34)$$

If $b=c$, the system shown in Fig. 1a is periodic and there is no local level. We shall show that this level appears immediately b deviates from c, no matter how small the deviation. It is clear from Eq. (34) for a fixed value of $k_\parallel$ that the spectra $\varepsilon_1(k_z)$ and $\varepsilon_2(k_z)$ for the right- and left-hand halves of a crystal are related by $\varepsilon_1(k)=\varepsilon_2(-k)$; near the edge of an energy band we have

$$\varepsilon_1(k)=E_0+\beta(k-k_0)^2, \quad \varepsilon_2(k)=E_0+\beta(k+k_0)^2. \quad (35)$$

We shall substitute in Eq. (23) the following expressions:

$$\varphi(z)=\bar{\varphi}(z)e^{iu(z)}, \quad u(z)\to k_0|z|, \ |z|\to\infty. \quad (36)$$

the function $\bar{\varphi}(z)$ varies slowly and we can expand Eq. (23) in terms of gradients:

$$W(z)\bar{\varphi}(z)+\alpha(z)\bar{\varphi}'(z)-\beta(z)\bar{\varphi}''(z)=E\bar{\varphi}(z), \quad (37)$$

where

$$W(z)=\sum_{z'}\bar{J}_{zz'}, \quad \alpha(z)=\sum_{z'}(z'-z)\bar{J}_{zz'},$$
$$\beta(z)=-\sum_{z'}\frac{(z'-z)^2}{2}\bar{J}_{zz'}, \quad (38)$$
$$\bar{J}_{zz'}=J_{zz'}\exp[iu(z')-iu(z)].$$

Comparing the spectrun of Eq. (37) at large distances from a defect with the spectrum given by Eq. (35), we find that in the limit $|z|\to\infty$

$$W(z)\to E_0, \ \alpha(z)\to 0, \ \beta(z)\to\beta. \quad (39)$$

Separating from $W(z)$, $\alpha(z)$, and $\beta(z)$ the asymptotes of Eq. (39), transferring the corresponding terms to the right-hand side of Eq. (37) and introducing a Green function $G_E(z-z')$ for the right-hand part, we obtain

$$\bar{\varphi}(z)=G_E(z)[W\bar{\varphi}(0)+A\bar{\varphi}'(0)+B\bar{\varphi}''(0)], \quad (40)$$

where

$$W=\sum_z[W(z)-E_0], \quad A=\sum_z\alpha(z), \quad B=\sum_z[\beta-\beta(z)]. \quad (41)$$

Equation (40) yields the following expression describing a local level:

$$1=WG_E(0)+AG_E'(0)+BG_E''(0). \quad (42)$$

If $|b-c|\ll c$, then the constants W, A, and B in the above expression are small. Since out of all three functions $G_E(0)$, $G_E'(0)$, and $G_E''(0)$ only the first diverges in the limit $E\to E_0$, we need retain only the first term on the right-hand sides of Eqs. (40) and (42); then these equations become identical with the corresponding equations describing a scattering defect [see Eq. (26)].

The expression for the constant W in terms of the overlap integrals is obtained from Eq. (38) and in the lowest order in $b-c$ it becomes

$$W=\sum_{z,z'\geqslant 0}[J_{zz'}-J_{z'-z}^{(0)}]+\sum_{z,z'\leqslant 0}[J_{zz'}-J_{z-z'}^{(0)}]-[J_{00}-J_0^{(0)}]$$
$$+\sum_{z\cdot z'<0}[J_{zz'}-J_{z'-z}^{(0)}]. \quad (43)$$

Here, $u(z)$ can be $k_0|z|$ because the difference in W associated with different selections of $u(z)$ is a quantity of a higher order of smallness. If we ignore the lattice deformations, we find that

$$J_{zz'}=J_{z'-z}^{(0)} \text{ for } z,z'\gtrsim 0, \qquad J_{zz'}=J_{z-z'}^{(0)} \text{ for } z,z'\leqslant 0 \quad (44)$$

and Eq. (43) simplifies to just the last term. When the overlap integrals decrease rapidly with distance (for the notation see Fig. 1a), we have

$$W=2(J_{bc}'-J_{bc}). \quad (45)$$

If we allow just for the nearest neighbors, we find that there is no local level.[15] When Eq. (45) is valid, a level splits off always because near the other edge of the band the constant W is the same.

It follows from the above discussion that the substitution of Eq. (36) reduces the problem of a twinning plane to that of some (strongly off-diagonal) scattering defect. Substituting Eq. (36) in the expression for $G_{\omega k_\parallel}$ of Eq. (14) and into the Gor'kov equation (15), we find that factors $\exp[iu(z)]$ cancel out in all the terms of this equation. Therefore, we obtain the theorem (formulated in Sec. 2) of equivalence of the superconducting properties of a twinning plane and a scattering defect in the case when the Fermi level is located near the edge of an energy band.

In general, the expressions for the Green functions are cumbersome (see the Appendix 2) and they differ considerably from those for a scattering defect, but all the properties formulated in Sec. 3 are retained.

5. TWO REGIMES OF LOCALIZATION OF THE ORDER PARAMETER

1. The temperature T_c of the transition to a localized superconductivity state is found from the condition of solubility of Eq. (18) with a kernel given by Eq. (19) [it is assumed that $V(z)=\text{const}$]. If the Fermi level is close to a Van Hove singularity so that $N_{2D}(\varepsilon)\propto\ln|\varepsilon|$, we can ignore the kernel $K_c(z,z')$ compared with $K_{\text{loc}}(z,z')$. In view of the degenerate nature of the kernel $K_{\text{loc}}(z,z')$ the equation obtained is readily solved by introducing Fourier components:

$$\Delta_q=\Delta_\varphi VN_{2D}(0)\ln\frac{1{,}14\omega_D}{T}\frac{(\varphi_0^2)_q}{1-K_0(q)},$$
$$\Delta_\varphi=\int dz\,\Delta(z)|\varphi_0(z)|^2. \quad (46)$$

The condition for self-consistency of these expressions is

$$1=VN_{2D}(0)\ln\frac{1{,}14\omega_D}{T}\int_{-\infty}^{\infty}\frac{dq}{2\pi}\frac{(\varphi_0^2)_q(\varphi_0^2)_{-q}}{1-K_0(q)}. \quad (47)$$

We shall divide the above integral into regions $|q|\lesssim\xi_0^{-1}$, $\xi_0^{-1}\lesssim|q|\lesssim\omega_D/v_F$ and $|q|\gtrsim\omega_D/v_F$; in the first region we shall assume that

$$K_0(q)=\lambda_0\left[\ln\frac{1{,}14\omega_D}{T}-\frac{1}{2}(\xi_0 q)^2\right], \quad \xi_0=\frac{v_F}{T_{c0}}\left[\frac{7\zeta(3)}{24\pi^2}\right]^{1/2}, \quad (48)$$

and in the third region we shall postulate that $K_0(q)=0$; the integral due to the second region is small. We thus obtain

$$1=\lambda_{loc}\ln\left(\frac{1{,}14\omega_D}{T}\right)\left\{\frac{1}{\lambda_0}\frac{a}{\xi_0}\left[\frac{T_{c0}}{2(T-T_{c0})}\right]^{1/2}+1\right\}, \quad (49)$$

where

$$\lambda_{loc}=VN_{2D}(0)a^{-1}, \quad a^{-1}=\int_{-\infty}^{\infty}|\varphi_0(z)|^4\,dz; \quad (50)$$

The quantity a is of the order of the localization radius of the function $\varphi_0(z)$. Then, Eq. (49) gives the asymptotes for the transition temperature T_c:[2)]

$$T_c=\begin{cases} T_{c0}\left[1+\frac{1}{2}\left(\frac{a}{\xi_0}\frac{\lambda_{loc}}{\lambda_0(\lambda_0-\lambda_{loc})}\right)^2\right], & \lambda_0-\lambda_{loc}\gg(a/\xi_0)^{1/2}, \quad (51a)\\ T_{c0}[1+(a/2^{1/2}\lambda_0^2\xi_0)^{2/3}], & |\lambda_0-\lambda_{loc}|\ll(a/\xi_0)^{1/2}, \quad (51b)\\ 1{,}14\omega_D\exp(-1/\lambda_{loc}), & \lambda_{loc}-\lambda_0\gg(a/\xi_0)^{1/2}. \quad (51c)\end{cases}$$

When λ_{loc} is varied, the transition between the asymptotes (51a) and (51b) occurs in a narrow range $\sim(a/\xi_0)^{2/3}$ near λ_0 (Fig. 5). In the limit $a/\xi_0\to 0$ the point λ_0 is the actual phase transition point. The nature of the solution

$$\Delta(z)=\text{const}\left\{a|\varphi_0(z)|^2+\frac{a\xi(T_c)}{\lambda_0\xi_0^2}\exp\left[-\frac{|z|}{\xi(T_c)}\right]\right\},$$
$$\xi(T)=\xi_0\left[\frac{T_{c0}}{2(T-T_{c0})}\right]^{1/2} \quad (52)$$

obtained from Eq. (46) can be used to demonstrate the physical meaning of a phase transition: if $\lambda_{loc}\approx\lambda_0$, a transition takes place from a state localized on the scale of $\xi(T)$ to a state localized at an atomic distance from a defect.

The solution (52) is an even function of z. A phenomenological analysis carried out by Andreev[16] demonstrates that a solution odd with respect to z can also exist and it has interesting properties. Such a solution is not obtained if $V(\mathbf{r})>0$ and if there are no magnetic effects; we then have $G_\omega(\mathbf{r},\mathbf{r}')=G_\omega(\mathbf{r}',\mathbf{r})$ and the kernel

$$K(\mathbf{r},\mathbf{r}')=V(\mathbf{r})T\sum_\omega|G_\omega(\mathbf{r},\mathbf{r}')|^2 \quad (53)$$

is a positive definite quantity. A Cooper instability appears in the eigenfunction of the kernel $K(\mathbf{r},\mathbf{r}')$ corresponding to the smallest characteristic value; this function has no nodes.[17]

2. If $N(0,z)=\text{const}$ and $V(z)\neq\text{const}$, the kernel $K(z,z')$ has a structure differing from that of Eq. (19):

$$K(z,z')=K_0(z-z')+\frac{\delta V(z)}{V}K_0(z-z'), \quad (54)$$

where $\delta V(z)=V(z)-V$. The second term is localized at $|z|\lesssim a$, $|z'|\lesssim\xi_0$; it is degenerate if we assume that $z=0$ in the argument of the kernel K_0. When Eq. (18) is solved by this method, the range of integration with respect to q in an expression of the (47) type is limited by the values $|q|\lesssim\xi_0^{-1}$ and a strongly localized regime does not appear. Then, the transition temperature T_c is described by[2]

$$\frac{T_c-T_{c0}}{T_{c0}}=\frac{1}{2}\left(\frac{\delta\lambda a}{\lambda_0^2\xi_0}\right)^2,$$
$$a\delta\lambda\equiv\int\delta\lambda(z)\,dz=\int N_0(0)\delta V(z)\,dz, \quad (55)$$

which confirms the estimate given by Eq. (1) and is valid if $\delta\lambda/\lambda_0\lesssim\xi_0/a$. Clearly, an increase in $V(z)$ near the boundary is of no qualitative importance and we shall therefore assume that $V(z)=\text{const}$.

3. Inclusion of the kernel $K_c(z,z')$ can be made by the methods described in the next section: the result given by Eq. (51c) is retained and instead of Eq. (51a) we obtain

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{2}\left(\gamma\frac{a}{\xi_0}\right)^2,$$
$$\gamma=\frac{(\lambda_0\bar\lambda_c+\overline{\lambda_c^2})(\lambda_0-\lambda_{loc})+\lambda_{loc}(\lambda_0+\lambda_c)^2}{\lambda_0^3(\lambda_0-\lambda_{loc})} \quad (56)$$

for $\lambda_{loc}>\lambda^*$, whereas we find that $\delta T_c=0$ for $\lambda_{loc}<\lambda^*$. The following notation is used here:

$$\lambda_c=\int\lambda_c(z)|\varphi_0(z)|^2\,dz,$$
$$\bar\lambda_c a=\int\lambda_c(z)\,dz, \quad \overline{\lambda_c^2}a=\int\lambda_c^2(z)\,dz. \quad (57)$$

A qualitative difference from Eq. (51a) is the appearance of a lower limit of existence of a localized superconductivity:

$$\lambda^*=\lambda_0\frac{\lambda_0\bar\lambda_c+\overline{\lambda_c^2}}{(\lambda_0\bar\lambda_c+\overline{\lambda_c^2})-(\lambda_0+\lambda_c)^2}\theta(-\lambda_0\bar\lambda_c-\overline{\lambda_c^2}). \quad (58)$$

By definition, we have $0\leqslant\lambda^*<\lambda_0$, and if $\lambda_{loc}>\lambda_0$, there is a localized superconductivity irrespective of the value of $\lambda_c(z)$; for low $\lambda_c(z)$ and $\lambda_{loc}(z)$ the condition $\lambda_{loc}>\lambda^*$ reduces to the requirement that the quantity of Eq. (12) should be positive.

6. DESCRIPTION OF A LOCALIZED SUPERCONDUCTIVITY

In the range of temperatures near T_{c0} we have to use the nonlinear Gor'kov equation (15). Substituting $G_{\omega k_\parallel}$ in the form of Eq. (16) and employing the obvious symbolic notation, we obtain

$$\Delta=[\bar G\Delta\bar G-\bar G\Delta\bar G\Delta\bar G\Delta\bar G+\dots]$$
$$+[G^{loc}\Delta G^{loc}-G^{loc}\Delta G^{loc}\Delta G^{loc}\Delta G^{loc}+\dots]. \quad (59)$$

The function $G^{loc}\propto 1/aT$ is localized for $|z|, |z'|\lesssim a$, whereas the function $\bar G\propto 1/a\varepsilon_F$ differs from the former in the absence of a defect for $|z|, |z'|\lesssim\xi_0$, and therefore the terms retained in Eq. (59) are equally important; on the other hand, the cross terms $\bar G^m(G^{loc})^n$ are of a higher order of smallness in a/ξ_0.

In view of Eq. (52) the solution should be sought in the

form of Eq. (11), where the function $\Delta_0(z)$ is localized for $|z| \lesssim a$, whereas $\psi(z)$ varies on a scale of $\xi(T)$. The first set of brackets in Eq. (59) contains terms with n factors Δ_0 and its order of smallness is $\sim (a/\xi_0)^n$ because of restrictions on the range of integration with respect to z_i; only the largest of these terms need to be retained. We shall show later that $\psi(z) \ll T_{c0}$ and that $\Delta_0(z)$ can be of the order of $\sim\psi(z)$ and $\sim T_{c0}$, so that we should retain terms of the lowest order in ψ, but include Δ_0 of every order. In the first set of brackets of Eq. (59) we have to retain terms

$$\tilde{G}\Delta_0\tilde{G}+\tilde{G}\psi\tilde{G}-\tilde{G}\psi\tilde{G}\psi\tilde{G}\psi\tilde{G} \tag{60}$$

(as usual, retention of a term cubic in ψ is related to the smallness of the coefficient in front of the term $\sim\psi$); it will be convenient to expand ψ in the second set of brackets of Eq. (59) later. The separation $\Delta = \Delta_0 + \psi$ can be made more specific as follows:

$$\Delta_0=(\tilde{G}\psi\tilde{G}-G^0\psi G^0)+[G^{loc}\Delta G^{loc}-G^{loc}\Delta G^{loc}\Delta G^{loc}\Delta G^{loc}+\ldots], \tag{61a}$$

$$\psi=G^0\psi G^0-G^0\psi G^0\psi G^0\psi G^0+\tilde{G}\Delta_0\tilde{G}. \tag{61b}$$

The function $G^0_{\omega k_\parallel}$ is given by Eq. (29) for a scattering defect and by Eqs. (A9)–(A11) with $\chi = -\alpha = \pi/2$ for a twinning plane. Consequently, we find that [see Eq. (21)]

$$\tilde{G}\psi\tilde{G}-G^0\psi G^0 \to \psi(0)\lambda_c(z)\ln(1.14\omega_D/T), \tag{62a}$$

$$\tilde{G}\psi\tilde{G}\psi\tilde{G}\psi\tilde{G}-G^0\psi G^0\psi G^0\psi G^0 \to -\psi(0)\frac{|\psi(0)|^2}{T_{c0}^2}\lambda_c(z)\frac{7\zeta(3)}{8\pi^2}, \tag{62b}$$

and Eq. (62b) can be ignored compared with Eq. (62a), as was already done in Eq. (61). In view of Eq. (62a) all the terms on the left-hand side of Eq. (61a) are localized at $|z| \lesssim a$, as assumed for $\Delta_0(z)$. The terms in the square brackets of Eq. (61a) are summed because of the degenerate nature of G^{loc}, to give the final expression

$$VN_{2D}(0)|\varphi_0(z)|^2 T\sum_{|\omega|<\omega_D}\int_{-\infty}^{\infty} d\varepsilon\frac{\Delta_\varphi}{\varepsilon^2+\omega^2+|\Delta_\varphi|^2}, \tag{63}$$

where Δ_φ is defined by Eq. (46).

Equation (61b) without the term cubic in ψ can be solved for ψ by adopting the Fourier representation. Since the term $\tilde{G}\Delta_0\tilde{G}$ does not contain the Fourier components with $|q| \gtrsim \xi_0^{-1}$, it is found that if $|T - T_{c0}| \ll T_{c0}$, the function $\psi(z)$ changes on the scale of $\xi(T)$ as assumed above. After expansion in gradients of ψ the term $\tilde{G}\Delta_0\tilde{G}$ can be replaced with the δ function and transformed by the sum rule of Eq. (21). Retention of these properties in the presence of a term cubic in ψ can be demonstrated by constructing an iteration series. We then obtain a system of equations describing a localized superconductivity:

$$\bar{\Delta}_0 = \lambda_{loc}\int_{-\omega_D}^{\omega_D} d\varepsilon\frac{\Delta_\varphi}{2(\varepsilon^2+|\Delta_\varphi|^2)^{1/2}}\operatorname{th}\frac{(\varepsilon^2+|\Delta_\varphi|^2)^{1/2}}{2T}, \tag{64}$$

$$\Delta_\varphi=\gamma_0\lambda_0\psi(0)+\bar{\Delta}_0,$$

$$\Delta_0(z)=\lambda_0^{-1}\psi(0)\lambda_c(z)+\bar{\Delta}_0 a|\varphi_0(z)|^2, \tag{65}$$

$$-\frac{1}{2}\xi_0^2\psi''(z)+\frac{T-T_{c0}}{T_{c0}}\psi(z)+\beta\frac{\psi(z)|\psi(z)|^2}{T_{c0}^2} = \delta(z)a[\gamma_0\bar{\Delta}_0+\gamma_1\psi(0)], \tag{66}$$

where the following notation is introduced

$$\gamma_0=\frac{\lambda_0+\lambda_c}{\lambda_0^2}, \quad \gamma_1=\frac{\lambda_0\bar{\lambda}_c+\overline{\lambda_c^2}}{\lambda_0^3}, \quad \beta=\frac{7\zeta(3)}{8\pi^2}. \tag{67}$$

Equation (66) is readily solved:

$$\psi(z)=\frac{T_{c0}(2t/\beta)^{1/2}}{\operatorname{sh}[(2t)^{1/2}(z+z_0)/\xi_0]}, \quad t=\frac{T-T_{c0}}{T_{c0}}. \tag{68}$$

The solution $\Delta(z)$ is fully described by Eqs. (65) and (68) if we know $\bar{\Delta}_0$ and $\psi(0)$, which can be found from Eq. (64).

If $\lambda_0 - \lambda_{loc} \gg (a/\xi_0)^{2/5}$, the quantity $\bar{\Delta}_0$ is proportional to $\psi(0)$ and the system can be described phenomenologically by the Buzdin–Bulaevskiĭ theory[2]:

$$\bar{\Delta}_0=\frac{\lambda_{loc}(\lambda_0+\lambda_c)}{\lambda_0(\lambda_0-\lambda_{loc})}\psi(0), \quad \psi(0)=T_{c0}\left(\frac{2(t_c-t)}{\beta}\right)^{1/2}. \tag{69}$$

However, the relationship between $t_c = \delta T_c/T_{c0}$ and $\delta\lambda$ becomes more complex [see Eq. (56)].

If $\lambda_{loc} - \lambda_0 \gg (a/\xi_0)^{2/3}$, the theory of Buzdin and Bulaevskiĭ[2] is even phenomenologically invalid: in the Ginzburg–Landau equation (66) in addition to the term $\sim\psi(0)\delta(z)$ there is also a const $\delta(z)$. The origin of this term is attributed in the phenomenological method of Andreev[16] to the existence of a two-dimensional order parameter Δ_0 and the presence in the surface energy of terms of the $\Delta_0\psi^*(0)$ type. The quantities $\bar{\Delta}_0$ and $\psi(0)$ are related to the microscopic parameters by

$$\bar{\Delta}_0=\begin{cases}2\omega_D\exp(-1/\lambda_{loc}), & \lambda_{loc}\gg\lambda_0\\ \dfrac{T_{c0}}{\lambda_0}\left(\dfrac{\lambda_{loc}-\lambda_0}{\beta}\right)^{1/2}, & \lambda_{loc}-\lambda_0\ll\lambda_0,\end{cases} \quad \psi^{(0)}=T_{c0}\left(\frac{\tau/\beta}{t/\tau+[1+(t/\tau)^2]^{1/2}}\right)^{1/2}, \tag{70}$$

where the parameter τ governing the temperature interval δT_{eff} of existence of a localized superconductivity is

$$\tau=\frac{\delta T_{\text{eff}}}{T_{c0}}=\gamma_0\beta^{1/2}\frac{\bar{\Delta}_0}{T_{c0}}\frac{a}{\xi_0}. \tag{71}$$

7. PERIODIC STRUCTURES

We shall now consider a system of periodically distributed planar defects separated by a distance $L_0 \gg a$. The Green function $G_{\omega k_\parallel}$ and the order parameter $\Delta(z)$ are now

$$G_{\omega k_\parallel}(z,z')=\bar{G}_{\omega k_\parallel}(z,z')+\sum_{z_i}G^{loc}_{\omega k_\parallel}(z-z_i,z'-z_i), \tag{72}$$

$$\Delta(z)=\psi(z)+\sum_{z_i}\Delta_0(z-z_i), \tag{73}$$

where z_i are the coordinates of the defects and $G^{loc}_{\omega k_\parallel}$ is defined by Eq. (16). Repeating the discussion given in Sec. 6,

we obtain a system of equations of the (61) type; in general, the quantity $\tilde{G}-G^0$ does not split into a sum of contributions of the individual defects, but the results contain only the quantity $\lambda_c(z)$ [Eq. (62)], which has this property, so that the only change needed in the system (64)–(66) is the replacement of $\delta(z)$ with a sum of the functions $\delta(z-z_i)$.

Linearization of the system yields an equation for the determination of T_c:

$$1=\lambda_{loc}\ln\left(\frac{1.14\omega_D}{T}\right)\left\{1+\lambda_0\gamma_0^2\left[-\gamma_1+\frac{\xi_0^2}{a\xi(T)}\,\mathrm{th}\,\frac{L_0}{2\xi(T)}\right]^{-1}\right\}, \tag{74}$$

which for $L_0\gg\xi(T_c)$ reduces to an equation for an isolated defect, whereas for $L_0\ll\xi(T_c)$, it yields

$$T_c=\begin{cases} T_{c0}[1+\gamma a/L_0], & \lambda_0-\lambda_{loc}\gg(a/L_0)^{1/2} \\ T_{c0}[1+\gamma_0(a/L_0)^{1/2}], & |\lambda_0-\lambda_{loc}|\ll(a/L_0)^{1/2}. \\ 1.14\omega_D\exp(-1/\lambda_{loc}), & \lambda_{loc}-\lambda_0\gg(a/L_0)^{1/2} \end{cases} \tag{75}$$

If $\lambda_{\mathrm{loc}}\gtrsim\lambda_0$ the characteristic range of temperatures where a localized superconductivity can be observed is governed by the following quantity in the case of periodically distributed defects:

$$\tau_\infty\sim\tau[\xi(\tau)/L_0]^{2/3},\quad L_0\ll\xi(\tau), \tag{76}$$

and for two defects separated by a distance L_0, this range is described by

$$\tau_2=2\tau,\quad L_0\ll\xi(\tau). \tag{77}$$

In the interpretation of the experimental results (Fig. 5) we must bear in mind that δT_{eff} has a quantitative meaning only when we compare situations in which the temperature dependences of the physical quantities are of the same type: for this reason we can extend the results of Eqs. (76) and (77) to the range $L_0\gtrsim\xi(\tau)$ and find the coefficient in (76).

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APPENDIX 1

MODIFICATION OF THE BCS EXPRESSION NEAR A VAN HOVE SINGULARITY

Substituting into the self-consistency equation of the BCS theory

$$1=V\int_{-\omega_D}^{\omega_D}N(\varepsilon)\frac{d\varepsilon}{2\varepsilon}\,\mathrm{th}\,\frac{\varepsilon}{2T} \tag{A1}$$

the density of states in the form $N(0)\ln(J/|\varepsilon|)$ and assuming that $\lambda_0=VN(0)$, we obtain

$$\frac{1}{\lambda_0}=\frac{1}{2}\left(\ln\frac{\omega_D}{T_c}\right)^2+\ln\frac{1.14J}{\omega_D}\ln\frac{\omega_D}{T_c}$$

$$+\ln 1.14\cdot\ln\frac{J}{\omega_D}+\int_0^\infty\frac{(\ln\varepsilon)^2\,d\varepsilon}{4\,\mathrm{ch}^2(\varepsilon/2)}. \tag{A2}$$

Retaining in turn one of the two logarithmic terms, we find that

$$T_c\sim\begin{cases}\omega_D\exp[-(2/\lambda_0)^{1/2}], & \ln(\omega_D/T_c)\gg\ln(J/\omega_D), \\ \omega_D\exp[-1/\lambda_0\ln(J/\omega_D)], & \ln(\omega_D/T_c)\ll\ln(J/\omega_D).\end{cases}$$

(A3)

(A4)

The result given by Eq. (A3) was obtained in Refs. 18 and 19 and it is valid only in the range $T_c\lesssim 1$ K, which is of no interest from the point of view of the high-temperature superconductivity. At values of T_c which are not too low, we can obtain estimates using Eq. (A4) representing the usual BCS expression for the case with a Van Hove singularity, truncated on the ω_D scale. The asymptotes of Eqs. (A3) and (A4) are not very accurate and Eq. (A2) can yield also a general expression

$$T_c=1.14J\exp(-\{2/\lambda_0+[\ln(J/\omega_D)]^2-1.31\}^{1/2}). \tag{A5}$$

Dzyaloshinskiĭ[19] demonstrated that when a Van Hove singularity is associated with a self-intersection of a two-dimensional Fermi surface at a near-normal angle, an investigation of the range $1\sim\lambda_0[\ln(\omega_D/T)]^2$ requires summation of a "parquet" pattern. This is important only in the case of anomalously small values of λ_0, because otherwise the terms $\sim\ln(\omega_D/T_c)\ln(J/\omega_D)$ predominate and the BCS expression applies.

APPENDIX 2

GREEN FUNCTION OF A TWINNING PLANE

In view of the mirror synmetry, the function $\varphi(z)$ is

$$\varphi(z)=\begin{cases}A|v_1|^{-1/2}e^{ik_1z}+B|v_2|^{-1/2}e^{ik_2z}, & z>0 \\ C|v_1|^{-1/2}e^{-ik_1z}+D|v_2|^{-1/2}e^{-ik_2z}, & z<0\end{cases} \tag{A6}$$

where k_α are the solutions of the equation $\varepsilon_1(k)=E$ and we also have $v_\alpha[\partial\varepsilon_1(k)/\partial k]_{k=k_\alpha}$. The coefficients A, B, C, and D are related by a unitary matrix which, after allowance for the mirror symmetry, becomes

$$\begin{pmatrix}B\\D\end{pmatrix}=\begin{pmatrix}e^{i\alpha}\cos\chi & ie^{i\alpha}\sin\chi\\ ie^{i\alpha}\sin\chi & e^{i\alpha}\cos\chi\end{pmatrix}\begin{pmatrix}A\\C\end{pmatrix}. \tag{A7}$$

The boundary conditions at the points $z=\pm L/2$ imply the absence of transmitted waves outside the sample:

$$\begin{aligned}A\exp(ik_1L/2)&=B\exp(ik_2L/2+i\varphi),\\ C\exp(ik_1L/2)&=D\exp(ik_2L/2+i\varphi).\end{aligned} \tag{A8}$$

If we obtain the eigenfunctions and the eigenvalues and calculate the sum over s in Eq. (14) for large values of z and z', then for $z>0$, $z'>0$ we obtain

$$\begin{aligned}\tilde{G}_{\omega k_\parallel}(z,z')=&G^{(1)}_{\omega k_\parallel}(z-z')\\ &-i\,\mathrm{sgn}\,\omega\frac{\cos\chi}{|v_1v_2|^{1/2}}\Big\{\exp[i(\alpha+k_2z-k_1z')]\\ &\times\exp\left[-\left|\omega\left(\frac{z}{v_2}-\frac{z'}{v_1}\right)\right|\right]\theta\left(\omega\left(\frac{z}{v_2}-\frac{z'}{v_1}\right)\right)\\ &+\exp[i(-\alpha+k_1z-k_2z')]\\ &\times\exp\left[-\left|\omega\left(\frac{z}{v_1}-\frac{z'}{v_2}\right)\right|\right]\theta\left(\omega\left(\frac{z}{v_1}-\frac{z'}{v_2}\right)\right)\Big\},\end{aligned} \tag{A9}$$

$$G^{(1)}_{\omega k_\parallel}(z-z') = -i \operatorname{sgn}\omega \sum_{\alpha=1,2} \frac{\exp[ik_\alpha(z-z')]}{|v_\alpha|} \times \exp\left(-\left|\omega\frac{z-z'}{v_\alpha}\right|\right)\theta\left(\omega\frac{z-z'}{v_\alpha}\right). \quad \text{(A10)}$$

If $z>0$, $z'<0$, we find that

$$\bar{G}_{\omega k_\parallel}(z,z') = \operatorname{sgn}\omega \frac{\sin\chi}{|v_1v_2|^{1/2}}\left\{\exp[i(\alpha+k_2z+k_1z')] \times \exp\left[-\left|\omega\left(\frac{z}{v_2}+\frac{z'}{v_1}\right)\right|\right] \times \theta\left(\omega\left(\frac{z}{v_2}+\frac{z'}{v_1}\right)\right) - \exp[i(-\alpha+k_1z+k_2z')] \times \exp\left[-\left|\omega\left(\frac{z}{v_1}+\frac{z'}{v_2}\right)\right|\right] \times \theta\left(\omega\left(\frac{z}{v_1}+\frac{z'}{v_2}\right)\right)\right\}. \quad \text{(A11)}$$

The other cases are obtained from the relationship $G_{\omega k_\parallel}(z,z') = G_{\omega k_\parallel}(-z,-z')$.

[1)]Such a splitting is not identical with the division of the order parameter into "two-dimensional" and "three-dimensional" in Ref. 5; the latter appear in Ref. 5 as components of a vector and not in a sum.

[2)]The results given by the system (51) are identical with those obtained in Ref. 5, where however they are expressed in terms of phenomenological parameters. The result $\delta T_c \sim T_{c0}$ is obtained in Ref. 6 without allowance for the contribution of Tamm levels. The source of error there is the incorrect nature of the oscillatory factor in the second term in Eq. (A3) for $G_\omega(x,x',\mathbf{k})$ in Ref. 6, so that the constant L_0 in the correct expression (10) is found to be $L_0 \sim \xi_0$. In reality, the expression for L_0 obtained by the sum rule of Eq. (21) transforms into an integral $\int \lambda_c(z)\,dz \sim a$.

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