Anomalies in the properties of tunneling and Josephson junctions in the vicinity of a Lifshits topological transition

A. A. Varlamov, A. V. Pantsulaya, and M. V. Fistul'

Moscow Institute of Steel and Alloys

(Submitted 8 January 1987)
Zh. Eksp. Teor. Fiz. **93**, 701–708 (August 1987)

We investigate the behavior of the I–V characteristics of a normal tunneling contact, and the critical current of a Josephson *S–N–S* junction, in the vicinity of a point where there is a change in the topology of the metal Fermi surface, for finite temperature and impurity concentration. We show that by studying anomalies in the I–V characteristics of tunneling contacts, we can evaluate the singular behavior of the electronic density of states near the topological transition; likewise, critical-current anomalies of the *S–N–S* contact let us study the behavior of the relaxation time.

1. Recently, the kinetic properties of metals near the electronic topological transitions (ETT) predicted by I. M. Lifshits[1] have been widely studied, both theoretically and experimentally. Anomalies have been observed in the thermoelectric power, conductivity, absorption coefficient of sound and other physical characteristics of the alloys $Li_{1-x}Mg_x$, $Cd_{1-x}Mg_x$, and BiSb, as well as in whiskers of Bi and Al[2–7], as the topology of the Fermi surfaces of these systems changes. The experimental data agrees fairly well with model theoretical calculations.[8–15]

Upon first examination, it seems that the primary contributions to the singular part of the kinetic coefficients must come from anomalies in the density of states near special points in momentum space (e.g., points where a "bridging section" is broken, producing a gap). However, the kinetic coefficients are proportional to the squared electron velocity as well as the density of states; the former vanishes near a special point and thereby compensates for the corresponding singularity coming from the density of states.[13] From this we conclude that in real systems, anomalies in the characteristics listed above occur because of a singularity in the electronic relaxation time, which behaves as an inverse square-root near the ETT. This singularity comes about because electrons can reach the vicinity of the singular point from everywhere on the Fermi surface as a result of scattering, a fact which also applies to the inverse processes. The second section of this paper is devoted to a detailed analysis of anomalies in the relaxation time for various types of transitions.

In addition to investigating the kinetic properties of metals near an ETT, there is much interest in studying the characteristics of tunnelling into these metals; such characteristics provide information about singularities in the metal electronic spectra.[15–18] Thus, if a tunneling contact is made whose electrodes (or at least one of them) undergo an ETT, it is possible to derive information about the behavior of the single-particle states near this transition from the corresponding I–V characteristics, taking into account "smearing" of the transition induced by finite temperatures and impurity concentrations.

On the other hand, by studying the dependence of the Josephson current on the parameter z which characterizes how close the metal is to the transition, we can determine the electronic relaxation-time singularities within the *S–N–S* when the N metal layer undergoes an ETT. The third and fourth section of this paper are devoted to these questions.

2. Changes in the Fermi-surface topology of real metals and alloys can occur in many different ways: the formation or disruption of "bridge" sections, the appearance or disappearance of new "sheets" (disconnected sections), etc. In the "broken-bridge" ETT model presented earlier in Refs. 11, 12, the Fermi surface was taken to be a hyperboloid of revolution, so that the dispersion law had the form

$$\varepsilon(\mathbf{p})-\mu=\mathbf{p}_\perp^2/2m_\perp-p_x^2/2m_x-z \qquad (1)$$

($z=\mu-E_c$, where E_c is the critical value of the energy corresponding to an ETT at $T=0$ and in the absence of impurities; $\mathbf{p}=\{p_x,\mathbf{p}_\perp\}$ is the electron momentum, μ is the chemical potential), The following expression was obtained for the relaxation time of an electron due to impurity scattering:

$$\tau^{-1}(\omega,z)=2\,\mathrm{Im}\,\Sigma^R(\omega,z)=\tau_0^{-1}[1-\delta(z+\omega)/2], \qquad (2)$$

where $\Sigma^R(\omega,z)$ is the self-energy part of the electronic Green's function averaged over the impurity positions.

Here,

$$\delta(x)=2^{1/2}[[{}^1/_4\tau^2\varepsilon_0^2+x^2/\varepsilon_0^2]^{1/2}-x/\varepsilon_0]^{1/2},$$

where τ_0 is the relaxation time of electrons due to impurities far from the ETT, $\varepsilon_0=p_{x0}{}^2/2m_x$, p_{x0} is the limiting value of the longitudinal momentum,[11] and ω is the energy of the electronic state under discussion measured from the level of the chemical potential.

Expression (2) was obtained on the basis of a one-band model in which the ETT formally corresponds to a transition from a two-sheeted ($z<0$) hyperboloid to a one-sheeted ($z>0$) hyperboloid. As is clear from (2), the relaxation time is finite, while the primary contribution to τ_0 is determined by scattering processes which take electrons from peripheral states of the Fermi surface ($p\sim p_{x0}$) into the same types of states [process 1 in Fig. 1(a)]. The small square-root correction $\tau_0\delta(z+\omega)/2$, which also describes how the kinetic coefficients vary close to the ETT, comes from scattering processes which take electrons from the peripheral regions into the singular region of the bridge (the vicinity of the point $\mathbf{p}=0$), and conversely [process 2 in Fig. 1(a)].

It must be pointed out that the finiteness of τ at the transition point can be proved without reference to any special features of a given model. Thus, e.g., in the "sheet-generation" type of ETT, the new sheet always appears near a rather large pre-existing section of the Fermi surface [Fig.

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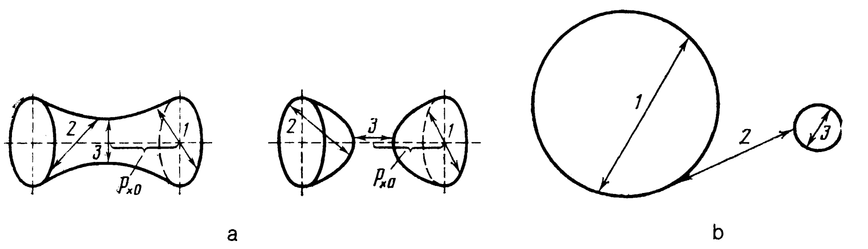

FIG. 1. Topological transitions: type a is the "broken bridge," type b is the "sheet generation." Because of scattering processes, 1—electrons arrive at the periphery of the Fermi surface from other peripheral regions; 2—electrons arrive in the vicinity of the Fermi surface singular point from peripheral regions; 3—electrons remain at the limits of the singular regions of the Fermi surface. Here p_{x0} is the limiting value of longitudinal momentum, $\varepsilon_0 = p_{x0}^2/2m_x$

1(b)] except for the case of a metal-insulator transition; an example of this is the overflow of electrons from two ellipsoids into a third in $Bi_{0.1}Sb_{0.9}$.[4] Therefore, just as in the case of the broken bridge, comparatively low-probability scattering processes involving a small group of electrons (processes 2, 3) are superposed on normal electron scattering processes which take electrons across the extended (large) section of the Fermi surface (process 1). In this case the relaxation time for electrons due to impurities is determined by a sum of the probabilities of all three processes, and is found to be finite. The proximity of the system to the ETT, as also in the case of a broken bridge, affects the relaxation time by introducing a small square-root correction.

3. Let us first consider a symmetric tunneling contact, both of whose electrodes undergo an ETT at the same time. The tunneling current which flows through the contact is determined by the expression[19]:

$$I(V)=\frac{2\pi^2}{em_\perp^2 p_{x0}^2 R_N}\int d\omega\left[\operatorname{th}\frac{\omega+eV}{2T}-\operatorname{th}\frac{\omega}{2T}\right]\cdot\int\frac{d^3\mathbf{p}}{(2\pi)^3}\operatorname{Im}G^R(\mathbf{p},\omega+eV)\int\frac{d^3\mathbf{k}}{(2\pi)^3}\operatorname{Im}G^R(\mathbf{k},\omega),\qquad(3)$$

where R_N is the ohmic resistance of the contact; the one-electron Green's function for the spectrum (1), taking into account scattering processes, was found earlier[11]:

$$G^R(\mathbf{p},\omega)=\left[\omega+z-\frac{\mathbf{p}_\perp^2}{2m_\perp}+\frac{p_x^2}{2m_x}+\frac{i}{2\tau(\omega,z)}\right]^{-1}.\qquad(4)$$

After coupling the imaginary part of the Green's function, integrated over momentum, with the self-energy part by using the self-consistency equation,[11] we are led to the following expression for the tunneling current

$$I(V)=\frac{2\tau^2}{eR_N}\int_{-\infty}^{\infty}d\omega\left[\operatorname{th}\frac{\omega+eV}{2T}-\operatorname{th}\frac{\omega}{2T}\right]\times\operatorname{Im}\Sigma^R(\omega+eV)\operatorname{Im}\Sigma^R(\omega).\qquad(5)$$

Differentiating expression (5) with respect to the voltage V in order to evaluate the additional differential contact resistance δR_{AN} which arises from the closeness of the system to ETT, we find

$$\frac{\delta R_{AN}}{R_N}=\frac{R(V)}{R_N}-1=\frac{1}{8T}\int_{-\infty}^{\infty}\frac{d\omega}{\operatorname{ch}^2(\omega/2T)}[\delta(\omega-eV+z)+\delta(\omega+eV+z)]=\left(\frac{T}{2\varepsilon_0}\right)^{1/2}\left\{F\left(\frac{z+eV}{2T}\right)+F\left(\frac{z-eV}{2T}\right)\right\}\qquad(6)$$

where

$$F(\xi)=2^{-1/2}\int_{-\infty}^{\infty}\frac{dx}{\operatorname{ch}^2x}\{[(2T\tau)^{-2}+(x+\xi)^2]^{1/2}-(x+\xi)\}^{1/2}.\qquad(7)$$

Expression (6) describes the behavior of the differential resistance of a symmetrical tunneling contact, both of whose electrodes undergo an ETT at finite temperatures and in the presence of electrons scattered by impurities.

In the case of a low impurity concentration ($T\tau\gg1$), the asymptotic form of the integral $F(\xi)$ takes the form

$$F(\xi)=\begin{cases}2|\xi|^{1/2}, & \xi\ll-1\\ \pi^{1/2}[\zeta(1/2)(1-2^{-1/2})+\xi\zeta(-1/2)(4-2^{1/2})], & |\xi|\ll1\\ (\pi/2)^{1/2}e^{-2\xi}, & 1\lesssim\xi\lesssim\ln T\tau\\ (4T\tau)^{-1}\xi^{-1/2}, & \xi\gg\ln T\tau\end{cases}\qquad(8)$$

Analysis of expression (6) shows that for $z\gtrsim0$ the function $R(V)$ has only a weakly expressed minimum at $V=0$ [Fig. 2(a)]. In the negative-z region this function is found to be considerably less trivial: even for $z\lesssim z^*=-1.1T$, the minimum at $V=0$ which occurred for $z\gtrsim0$ has gradually been converted into a maximum [Fig. 2(b)], while at specific values of voltage $\pm V_{\min}$ there appear two characteristic minima in the function $R(V)$ [Fig. 2(c)]. In the case $z\ll-T$, the positions of these minima can be found analytically from the condition (6) that the function $R(V)$ be at an extremum; taking advantage of the asymptotic representation for the function $F(\xi)$:

$$\pm eV_{min}=\begin{cases}|z|+(T/2)\ln(2\pi|z|/T), & T\ll|z|\ll T(T\tau)^2,\\ |z|+(|z|/8\tau^2)^{1/3}, & |z|\gg T(T\tau)^2.\end{cases}\qquad(9)$$

Let us now turn to the case of an impure metal ($T\tau\ll1$). Then the slowly-varying function δ in equation (6) can be taken outside the integral sign, because $\operatorname{ch}^{-2}(\omega/2T)$ varies much more rapidly than the second factor; after doing this, it is easy to show that

$$\delta R_{AN}/R_N=1/2[\delta(z+eV)+\delta(z-eV)].\qquad(10)$$

The function $\delta(x)$ which enters into this expression was de-

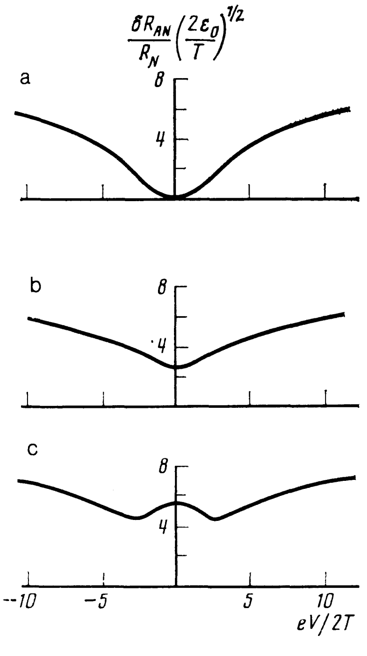

FIG. 2. Dependence of the relative contribution to the differential resistance of a tunneling contact on voltage for constant parameter values z: (a) $z=4T$, (b) $z=-1.1T$, (c) $z=-4T$.

termined above; in the interest of clarity we will write it here in asymptotic form:

$$\delta(x)=\varepsilon_0^{-1/2}\begin{cases}2|x|^{1/2}, & -\tau x\ll 1,\\ (1-x\tau)\tau^{-1/2}, & \tau|x|\ll 1,\\ 1/2\tau x^{1/2}, & \tau x\gg 1.\end{cases} \qquad (11)$$

We see that, as in the case of a pure metal, for sufficiently large $|z|$ ($-\tau z\ll 1$) the function $R(V)$ has two subsidiary minima at the voltages

$$\pm eV_{min}=|z|+(|z|/8\tau^2)^{1/3}. \qquad (12)$$

We note that this expression accurately reproduces the second asymptotic form for $\pm eV_{\min}$ in equation (9) when $|z|$ is large. This implies that even in the case $T\tau\gg 1$ we cannot ignore impurity scattering anywhere, because of the exponential decrease in the function $F(\xi)$ for $1\lesssim\xi\lesssim\ln T\tau$. Even in a pure metal ($T\tau\gg 1$), for sufficiently large $|z|$ ($|z|>T^3\tau^2$) the situation turns out to be fully analogous to the impure-metal case ($T\tau\ll 1$).

The appearance of these subsidiary minima in the function $R(V)$ has its origin in a phenomenon which we may call "electrical breakdown" of the Fermi surface, in analogy with the phenomenon of "temperature breakdown."[11] In essence, this phenomenon can be described as follows: as z increases from the region of large negative values, the closed-off Fermi surface approaches the edge of the Brillouin zone; if we apply a voltage $eV\sim|z|$ to the tunneling contact in this case, then in a sense this voltage "opens up" the Fermi surface, changing its connectivity and thereby causing an ETT. As z grows (i.e., for $z\approx-\max[\tau^{-1}, T]$) these subsidiary minima gradually disappear, since in this region—even without an electric field, simply because of smearing of the Fermi surface due to temperature or impurities—the ETT is smeared out and begins earlier than it does at $T=0$.[11] In the positive-z region, the Fermi surface is already open, and applying an electric field does not change its topology. Therefore, the differential resistance shows no anomaly of any kind.

We now can draw some conclusions about the way the I–V characteristics change with temperature. At high temperatures, for $T\gg\tau^{-1}$ and when z belongs to the region of greatest interest, i.e., $-T(T\tau)^2<z<-T$, the I–V characteristic of the tunneling contact has the form chosen in Fig. 2(c). As the temperature decreases, according to (9) the subsidiary minima approach each other smoothly, remaining close to the points $eV_{\min}\sim\pm|z|$. When the temperature reaches $\sim\tau^{-1}$, a transition occurs to the case of an impure metal. The motion of the minima comes to an end, and they fade away at the position $eV_{\min}\approx|z|+(|z|/8\tau^2)^{1/3}$.

We now discuss the case of an asymmetric contact, one of whose electrodes is a normal metal while the other, under the influence of an external stimulus, undergoes an ETT. Here also the tunneling current flowing through the contact is determined by expression (3); however, we now identify one of the functions G^R as a normal-metal Green's function. Analogously, we obtain for the relative contribution to the differential resistance of the contact

$$\frac{\delta R_{AN}}{R_N}=\frac{1}{8T}\int_{-\infty}^{\infty}\frac{d\omega}{\mathrm{ch}^2(\omega/2T)}\delta(\omega-eV+z)=\left(\frac{T}{2\varepsilon_0}\right)^{1/2}F\left(\frac{z-eV}{2T}\right) \qquad (13)$$

[the asymptotic behavior of the function $F(\xi)$ in the pure and impure cases is determined by expressions (8), (7) and (11)].

We note that in contrast to (6), for this case the correction depends strongly on the sign of the voltage applied to the contact. In the region of large positive voltage ($eV\gg\max[T,\tau^{-1}]$) the contact resistance increases as a square root, while in the region of large negative voltage the resulting ETT correction falls off as $\sim(eV)^{-1/2}$. In this case we observe a kink in the dependence of the resistance on voltage, which occurs in the region $eV\sim z$, in agreement with the considerations discussed earlier regarding "electrical breakdown." In this case, when the voltage on the contact is changed, we can shift the transition; this changes the topological connectivity of the Fermi surface independent of the value of z.

4. We now turn to a discussion of another tunneling structure: a superconductor-metal-superconductor (S–N–S) contact whose metallic layer undergoes an ETT. It is the impure contact ($T\tau\ll 1$) which is most interesting here.

In order to calculate the critical current density of the S–N–S contact, we make use of results analogous to those obtained in Refs. 20, 21:

$$j_c(z)=Aj_c(\varepsilon_0)\sum_n(\omega_n^2+\Delta_1^2)^{-1/2}(\omega_n^2+\Delta_2^2)^{-1/2}\times\int_{-\infty}^{\infty}\frac{dq}{2\pi}e^{iqa}\Pi(q,\omega_n),$$

$$A=\frac{p_0\tau_0}{m_x}\left(\frac{\pi T\tau_0}{6}\right)^{1/2}\exp\left[\left(\frac{T}{T_1}\right)^{1/2}\right]\{(\pi^2T^2+\Delta_1^2)(\pi^2T^2+\Delta_2^2)\}^{1/2}, \qquad (14)$$

where the characteristic temperature is given by $T_1=p_0^2\tau_0/6\pi a^2m_x^2$, and a is the contact thickness. The quantities Δ_1 and Δ_2 which enter into this expression denote the superconducting gaps of the superconducting electrodes. Here $\Pi(q,\omega_n)$ is the polarization operator for electrons in the metallic layer averaged over the impurity positions, and $\omega_n = 2\pi T(n+1/2)$ is the Matsubara frequency for fermions. We note that expression (14) is correct only at high temperatures, $T \gg T_1$.

Analogously, [14] the polarization operator $\Pi(q,\omega_n)$ averaged over impurity positions in the layer can be expressed in terms of the single-electron Green's function:

$$\Pi(q,\omega_n)=J/(1-J),$$
$$J=\int \frac{d^3\mathbf{p}}{(2\pi)^3} G(\mathbf{p}_\perp, p_x+q, \omega_n) G(-\mathbf{p}_\perp, -p_x, -\omega_n) \frac{1}{4\pi\tau_0 p_{x0}} \tag{15}$$

(we have directed the hyperboloid axis perpendicular to the contact plane).

The single-electron Green's function entering into this expression corresponds to (4); however, it is evaluated at the Matsubara frequencies. Performing the integration in (15), we find

$$J=\left\{\frac{\tau}{ql\tau_0}\operatorname{arctg}\frac{lq}{1+2\omega_n\tau}-J_1\right\}, \tag{16}$$

where

$$J_1=\frac{1}{\pi(1+2\omega_n\tau)}\int_0^1 \frac{dt}{1+(qv_{x0}\tau)^2/(1+2\omega_n\tau)^2} \times \operatorname{arctg}\frac{1+2\omega_n\tau}{2\tau(z+\varepsilon_0 t^2)}, \tag{17}$$

here $l = p_{x0}\tau/m_x$ is the mean free path of an electron in the metallic layer far from the ETT; $v_{x0} = p_{x0}/m_x$.

The primary contribution to the integration over momentum in (14) comes from the region of small momentum, where, as was shown in Ref. 14, the integral J_1 has the form

$$J_1=\frac{1}{2(1+2\omega_n\tau)}\delta(z,0),$$
$$ql \leqslant \min\{(2\varepsilon_0\tau)^{1/2}, \ (\varepsilon_0/|z|)^{1/2}\}.$$

In this way, we obtain the following expression for the critical current of the contact:

$$j_c(z)=Aj_c(\varepsilon_0)\sum_n[(\omega_n^2+\Delta_1^2)(\omega_n^2+\Delta_2^2)]^{-1/2}/2\pi \cdot \int_{-\infty}^{\infty}\frac{e^{iqa}\,dq}{\omega_n\tau_0+\tau/\tau_0+(ql)^2/3+J_1(z)-1}. \tag{18}$$

This integral can be calculated using the explicit expression for τ [see (2)] and keeping the first terms in the sum over frequency [since the terms of the sum in (18) decrease exponentially as ω_n grows]:

$$j_c(z)=j_c(\varepsilon_0)\exp\{-2a(6\pi T\tau_0 m_x/\varepsilon_0)^{1/2}(1/\tau-1/\tau_0)\} = j_c(\varepsilon_0)\exp[(T/T_1)^{1/2}\delta(z)/2], \tag{19}$$

where the asymptotic behavior of the function $\delta(z)$ is determined by expression (11).

Thus, as a function of distance from the ETT, the critical current has a singularity which is far sharper (exponential) than the singularities in the kinetic properties discussed earlier (Refs. 8–15; see Fig. 3). This result has a simple physical explanation: Cooper pairs which traverse the layer of N-metal are scattered by impurities. In a Type 1 scattering process (Fig. 1), the momenta of the electrons which form a pair does not change in order of magnitude and is determined by the large value $p_0 \sim (2m\varepsilon_0)^{1/2}$. Therefore, such electrons tranverse the layer in almost the same way as the usual case (i.e., a metal without an ETT). However, for scattering of electrons in the N layer, Type 2 scattering processes are also possible (Fig. 1). As a result, electrons can then be scattered into the small-momentum region ($|\mathbf{p}| \sim 0$). Correspondingly, the "time in residence" of a Cooper pair made up of such slow electrons in the normal-metal layer increases markedly; because of this, the Cooper pair disintegrates, and does not contribute to the critical current of the Josephson contact.

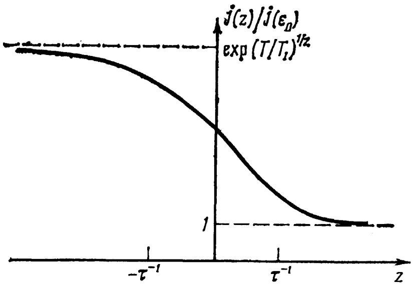

FIG. 3. Dependence of the critical current density on the parameter z which characterizes closeness of the S–N–S contact to the ETT.

At high temperatures ($T \gg \tau^{-1}$), the role of impurity scattering is unimportant, and during a transit time of the N layer, practically all the usual Cooper pairs can avoid conversion into slow ones. In this temperature region $j_c(z,T)$ is almost independent of the distance from the ETT, and coincides with $j_c(\varepsilon_0,T)$. As the temperature falls ($T \lesssim \tau^{-1}$), the "slowing down" mechanism mentioned earlier begins to make itself felt on the Cooper pairs in the N layer, and $j_c(z)$ begins to depend significantly on the degree of closeness to the ETT [Eq. (19)].

Thus, at temperatures $T \sim \tau^{-1}$ the dependence of the relative critical current density $j_c(z,T)/j_c(\varepsilon_0,T)$ has a smeared-out step whose magnitude $\exp[(T_1\tau_0)^{-1/2}\delta(z)]$ for some ratio $(\delta^2/(T_1\tau) \gg 1)$ can turn out to be quite sizeable.

5. In conclusion, let us formulate the basic results obtained in the paper:

1) The electronic relaxation time due to impurities at the ETT remains finite, and its value is determined primarily by scattering processes for which the singular region of momentum space, i.e., the region where the transition occurs, is irrelevant. The closeness to the ETT appears in $\tau(z)$ only through a weak square-root singularity which is caused by scattering of slow electrons by impurities, with their subsequent ejection to parts of the Fermi surface far from the singular part (likewise the inverse processes). However, it is this singularity which gives rise to the anomalies observed in the kinetic coefficients.

2) The relaxation time $\tau(z)$ can be directly extracted from the dependence of the critical current of an S–N–S Josephson contact on distance from an ETT which takes place in the normal metal layer under study. It was shown that the critical current in such a contact is extremely sensitive to the

ETT, and can itself vary in the vicinity of the transition by an order of magnitude. This fact is due to the possibility of unusual (i.e., compared to a normal metal) scattering of superconducting electrons when they tunnel through the normal layer, in the process of which the electrons enter the singular region and slow down. Their diffusion time in the layer thus increases significantly, destroying the Cooper correlation.

3) Study of the I–V characteristics of a tunneling contact whose electrons undergo an ETT allow us to ascertain the behavior of the density of states near the ETT. It was shown that as the closed Fermi surface approaches the edge of the Brillouin zone under the action of a voltage applied to the contact, the phenomenon of "electric breakdown" of the Fermi surface can occur, in which the connectivity of the latter decreases. This phenomenon is accompanied by characteristic minima in the I–V characteristics of the tunneling contact.

In conclusion, the authors express their profound gratitude to A. A. Abrikosov, B. L. Al'tshuler and M. I. Kaganov for their interest in the work.

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Translated by Frank J. Crowne