Generalized topological transition; the surface phase transition of order $2\frac{1}{2}$

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It is shown that a change in the local structure of the Fermi surface can lead to a singularity of the electronic part of the surface energy of a conductor. At zero temperature this singularity should be treated as a phase transition of order $2\frac{1}{2}$.

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As shown by I. M. Lifshitz[1] and observed in experiment (see Ref. 2 and the literature cited in both articles), a change in the connectivity of the Fermi surface (FS) leads to anomalous electronic characteristics of a metal. In Ehrenfest's terminology, these anomalies (at zero temperature T) should be regarded as phase transition of order $2\frac{1}{2}$. The transition takes place either when the FS acquires a new cavity, or when a neck is broken in it. In both cases the state density is

$$\nu(\varepsilon_F)=\frac{2}{(2\pi\hbar)^3}\oint_{\varepsilon(\mathbf{p})=\varepsilon_F}\frac{dS}{v},\quad \mathbf{v}=\nabla_{\mathbf{p}}\varepsilon \tag{1}$$

(the notation is standard[3]) has at the transition point a square-root singularity $\delta\nu(\varepsilon_F)\propto|\zeta|^{1/2}$, where $\delta=\varepsilon_F-\varepsilon_c$; at $\varepsilon=\varepsilon_c$ the equal-energy surfaces $\varepsilon(\mathbf{p})=\varepsilon$ change their topology, and this change affects a small vicinity of $\mathbf{p}$ space around the point $\mathbf{p}=\mathbf{p}_c$, at which the velocity $\mathbf{v}_c=(\partial\varepsilon/\partial\mathbf{p})_{\mathbf{p}=\mathbf{p}_c}=0$. This is precisely why an infinitesimal change of the FS manifests itself in measurable macroscopic characteristics of the metal.

The effect exerted on the sound damping coefficient Γ by a change in the local geometry of the FS without loss of its connectivity was investigated in Ref. 4, and the following was shown: reversal of the sign of one of the FS curvature radii (the appearance of a constriction—"waistline") or the reversal of the sign of both curvature radii (the appearance of a hollow—"crater" or "ravine") should manifest itself in an anomalous $\Gamma=\Gamma(\zeta)$ dependence, and ε_c should be taken to mean that value of the energy ε at which the ravine or the waistline give rise to a topological transition. This has served as the basis for introducing the concept "generalized topological transition," [1)] although it must be borne in mind that the state density (1) has no singularity at $\zeta=0$ in this case.

It will be shown below that a change in the local structure of the FS should lead, at $\zeta=0$, to a singularity of the surface density $\nu_\sigma(\varepsilon_F)$ of the electronic surface states and should manifest itself in the form of a surface phase transition or order $2\frac{1}{2}$. This means that the surface part of the free energy F_σ should contain (at $T=0$) a term proportional to $|\zeta|^{5/2}$. According to Ref. 6, $\nu_\sigma(\varepsilon_F)$ is expressed in the form of a contour integral:

$$\nu_\sigma(\varepsilon_F)=-\frac{2\sigma}{(4\pi\hbar)^2}\oint_{(C_n)}\frac{dl}{v},\quad \sigma=\frac{2V}{D}, \tag{2}$$

where V is the volume of the metallic plate and D is its thickness, while the contour C_n ("belt") is chosen to fit the condition that the Fermi-electron velocities be parallel to the plate surfaces:

$$\varepsilon(\mathbf{p})=\varepsilon_F,\qquad \mathbf{nv}=0, \tag{3}$$

$\mathbf{n}$ is the vector normal to the surface (Fig. 1). Naturally, in topological transitions, i.e., when the connectivity of the FS is changed, the surface density of states $\nu_\sigma(\varepsilon_F)$ also has singularities, even stronger ones than those of the volume density of states $\nu(\varepsilon_F)$. They are investigated by Nedorezov.[6] As can be seen from (2) and (3), however, for $\nu_\sigma(\varepsilon_F)$ to have a singularity it suffices to change the connectivity of the belt (3), and this can be done without changing in the connectivity of the FS if hollows (ravines) are produced on the surface (as a result of external action).

A topological change of the structure of the belt (3) can apparently occur in the general case in only two ways:

a) by formation (vanishing) of a new loop of the belt (Fig. 1b) and

b) by disruption (or formation) of a neck on the belt (Fig. 1d).

In the first case a hollow (ravine, crater; Fig. 1b) is produced on the FS, and the second the "watershed between two ravines" is eliminated (Fig. 1d). If the FS cavity has high symmetry (e.g., is a body of revolution), an external action can produce a nonlocal change of the FS. An example is the formation of a waist (Fig. 2), which is considered in Ref. 4.

Since the change of the belt topology is connected with its local restructuring, the anomalous part $\nu_\sigma(\varepsilon_F)=\nu_\sigma(\varepsilon_c+\zeta)$ (which we designate $\delta\nu_\sigma(\zeta)$) is deter-

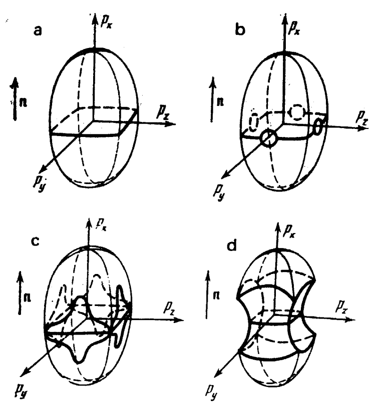

FIG. 1. Structure of "belt" on a FS at different values of ζ: a) $\zeta>0$; b) $\zeta_c<\zeta<0$; c) $\zeta=\zeta_c<0$; d) $\zeta<\zeta_c<0$.

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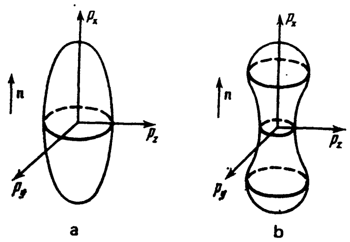

FIG. 2. Formation of a "waist on a FS with axial symmetry: (a) $\zeta>0$; (b) $\zeta<0$.

mined by integrating either over the small loop (case (a)) or over the section of the belt adjacent to the self-intersection point (case (b)). This enables us to take the velocity v from under the integral sign:

$$\delta\nu_\sigma(\zeta) = -\frac{2\sigma}{(4\pi\hbar)^2 v_c}\,\delta l(\zeta), \quad \delta l(\zeta) = \delta \oint_{(C_n)} dl, \tag{4}$$

where v_c is the velocity at the critical point $\mathbf{p}_c$ of the belt (at the point of creation of the belt in case (a); at the point of self intersection in case (b)).

As a rule the surfaces of a plate coincide with "good" crystallographic directions, and the vector $\mathbf{n}$ is by the same token directed along one of the symmetric directions (Figs. 1 and 2). In this case the critical point of the belt should be a point of increased symmetry of the FS.

We begin with formation of a ravine, assuming that the point $\mathbf{p}_c$ has a symmetry corresponding to a sixfold (or fourfold) axis perpendicular to the plane tangent to the FS at the point $\mathbf{p}_c$. This assumption [2)] allows us to parametrize the section of the FS near the point $\mathbf{p}_c$ chosen as the origin by using the symmetric form

$$\zeta = v_c p_z + (\zeta/2m\varepsilon_0)(p_x^2+p_y^2) + \eta(p_x, p_y), \tag{5}$$

where $\eta(p_x, p_y)$ is a homogeneous fourfold form. If p_z coincides with a sixfold axis, then

$$\eta(p_x, p_y) = (p_x^2+p_y^2)^2/4mp_0^2, \tag{6}$$

since it is impossible to set up an invariant combination of p_x and p_y of the required degree relative to rotation through 60°, other than $(p_x^2+p_y^2)^2$. The parameters ε_0 and p_0 are respectively of the order of ε_F and p_F, and if m is taken to be the mass of the free electron, the coefficients of $p_x^2+p_y^2$ and $(p_x^2+p_y^2)^2$ can be easily expressed in terms of the corresponding derivatives of the energy with respect to the quasi-momentum at $\mathbf{p}=\mathbf{p}_c$; they are written in the form assumed here for convenience in making the estimates (cf. Ref. 4). If p_z coincides with a fourfold axis, then

$$\eta(p_x, p_y) = \frac{(p_x^2+p_y^2)^2}{4mp_1^2} + \frac{p_x^2 p_y^2}{2mp_2^2}, \quad p_{1,2} \propto p_F. \tag{6'}$$

We direct the vector $\mathbf{n}$ along the x axis. To write the belt equation (3) it is necessary to add to (5) the equation

$$p_x\left(\frac{\zeta}{\varepsilon_0} + \frac{1}{p_0^2}(p_x^2+p_y^2)\right) = 0, \tag{7}$$

if Eq. (6) is valid, and the equation

$$p_x\left[\frac{\zeta}{\varepsilon_0} + \frac{p_x^2}{p_1^2} + \left(\frac{1}{p_1^2} + \frac{1}{p_2^2}\right)p_y^2\right] = 0, \tag{7'}$$

if Eq. (6') is valid. It can be seen from the last expressions that at $\zeta<0$ (we have assumed for the sake of argument $\varepsilon_0>0$) there is a "new" loop of the belt (this loop is absent at $\zeta>0$, and the belt is the intersection of the FS with the plane $p_x=0$). In the first case (Eq. (7)) the new belt is a circle of radius $p_0(|\zeta|/\varepsilon_0)^{1/2}$, and in the second (Eq. (7')) it is an ellipse with axes $\tilde{p}_x = p_1(|\zeta|/\varepsilon_0)^{1/2}$ and $\tilde{p}_y = \tilde{p}(|\zeta|/\varepsilon_0)^{1/2}$, $\tilde{p}^{-2} = p_1^{-2} + p_2^{-2}$. Since the surface density $\delta\nu_\sigma(\zeta)$ is proportional according to (4) to the length of the produced belt, it is clear that in both cases

$$\delta\nu_\sigma(\zeta) = \begin{cases} -\dfrac{4\pi\sigma m_c^*}{(4\pi\hbar)^2}\left(\dfrac{|\zeta|}{\varepsilon_0}\right)^{1/2}, & \zeta<0, \\ 0, & \zeta>0 \end{cases} \tag{8}$$

The effective mass $m^*_c = p_0/v_c$ for a circle, while for an ellipse it is written in the form of an elliptic function of the ratio p_1/p_2; in the general case $m^*_c \sim m$.

In order for the belt to experience disruption (or creation) of a neck, it is necessary that the function $\eta = \eta(p_x, p_y)$ in (5) have the structure

$$\eta(p_x, p_y) = (p_x^2 - p_y^2)^2/2mp_0^2. \tag{9}$$

The coefficients of p_x^2 and p_y^2 were chosen here equal in absolute value only for the sake of convenience: introduction of the factor ~ 1 does not change the results qualitatively. The equation of the anomalous section of the belt

$$p_x^2 - p_y^2 = -p_0^2\zeta/\varepsilon_0 \tag{10}$$

shows that at $\zeta=0$ the belt has a self-intersection point ($p_x=p_y=0$). Calculating the difference $l(\zeta)-l(0)$, we can easily show that

$$\delta l(\zeta) \approx -\beta p_0(|\zeta|/\varepsilon_0)^{1/2},$$

$$\beta = 2\sqrt{2}\int_0^\infty \frac{du}{(u^2+1)^{1/2}[(u^2+1/2)^{1/2}+(u^2+1)^{1/2}]} \approx 1.6$$

and consequently $\delta\nu_\sigma(\zeta)$ has square-root singularities on both sides of $\zeta=0$ (this is one of the differences between a surface and a volume transition, cf. Ref. 1):

$$\delta\nu_\sigma(\zeta) \approx \frac{2\sigma m_c^*}{(4\pi\hbar)^2}\,\beta\left(\frac{|\zeta|}{\varepsilon_0}\right)^{1/2}. \tag{11}$$

The infinite limit of the integral of the last formula is the consequence of the convergence of the integrand.

If the coefficients of p_x^2 and $-p_y^2$ in (9) were different, the coefficients of $(|\zeta|)^{1/2}$ on both sides of the transitions would also be different.

Figures 1a–1d show how a neck is produced on a FS as a result of two successive generalized topological transitions. Figure 3 shows the schematic dependence of the surface state density. If the FS is a body of revolution, a constriction (waist) can be produced as a result of one transition. The surface density of states undergoes in this case a finite jump equal to double the value of ν_σ at $\zeta=0$:

$$\delta\nu_\sigma(\zeta) = 2\nu_\sigma(\zeta=0),$$

inasmuch as the formation of the constriction produces two new belts, whose lengths at small value of ζ hardly differ

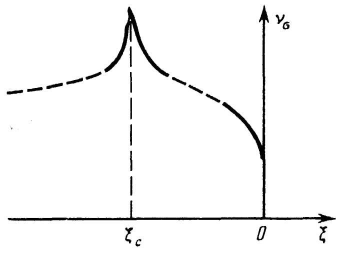

FIG. 3. Schematic variation of the surface state density ν_σ upon formation of a FS neck via two generalized topological transitions.

from the length of the original belt (Fig. 2).

The surface free energy is determined by the surface density of the states with the aid of the same formulas as the volume free energy is determined by the volume state density. There is therefore no need to calculate the anomalies of the surface thermodynamic characteristics in a phase transition of order $2\frac{1}{2}$ (Ref. 1). The only difference is that when the neck is broken at the belt (i.e., when the "watershed between two ravines" is eliminated), a singularity exists on each side of the transition.

A genearalized topological transition should be observed as a rule at a weaker action than a transition due to the change of the FS connectivity, although it need not necessarily precede it (if the FS contains a thin neck, the latter can "break" before the other sections of the FS sense any action). Experimental searches for the effects predicted here should be made for those metals for which an effect of pressure on the electronic energy spectrum has been observed (Bi, Sb, Cd, Zn) and others). In addition, the FS of a number of metals have quasicylindrical and quasiplanar sections (W, Mo, chalcogenides, and others). Clearly, a comparatively small action should lead to a change of their local structure. To be sure, it must be kept in mind that to observe a local change of the FS structure by spotting an anomaly of the surface energy it is necessary to choose correctly the orientation of the surfaces of the plate (of the vector **n**) relative to the crystallographic axes; a surface phase transition of order $2\frac{1}{2}$ can be observed only when the "belt" is restructured. Thus, when a convexity ("hill") is formed on a quasiplanar section of the FS, the vector **n** should be almost parallel to this section (cf. Ref. 4). Formation of a waist was observed (as revealed by oscillatory effects in a magnetic field) in Te when the degree of doping was changed,[7] and possibly in Bi under pressure.[8] It would be very interesting to observe for these metals anomalies of the thermodynamic characteristics at $H = 0$.

A change in the shape of the FS should naturally manifest itself also in the oscillatory part of the free energy, since the appearance (vanishing) of a ravine can alter the character of the interaction between the electrons and the surface of the sample on account of the appearance (vanishing) of a channel in multichannel specular reflection.[9] According to Slutskin and Kadigrobov[9] the multichannel character of the specular scattering is a source of quantum interference phenomena that complicate the oscillation spectrum.

We recall in conclusion that (according to Ref. 4) a generalized topological transition should lead to the onset of anomalies of the kinetic characteristics, and in particular to a sharp anisotropy of the ultrasound absorption coefficient. One should expect a change in the spectrum of the Sondheimer, Pippard, and de Haas–van Alphen oscillations, and in general anomalies of those electronic properties that are sensitive to the local structure of the FS (see Ref. 10).

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[1)] In Ref. 5, when considering the origin of the electron spectrum of Bi, Abrikosov and Fal'kovskiĭ have shown that deformation can change the Fermi surface from an ovaloid into a "dumbell."

[2)] The symmetry of the produced ravine is naturally independent of the orientation of the vector **n**, whose direction determines the symmetry of the belt (3).

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