The Effect of Changes in the Topology of the Fermi Surface on Superconducting Properties

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Submitted August 3, 1971

Zh. Eksp. Teor. Fiz. **62**, 1118–1130 (March, 1972)

The dependence of the superconducting transition temperature T_c on the Fermi energy ϵ_F is investigated in that range of values $\epsilon_F \approx \epsilon_c$ where changes in the topology of the Fermi surface occur. The change of the superconducting transition temperature due to the change of the Fermi energy is found for the case of a smooth dependence of the amplitude of the effective electron-electron attraction on the energy. The dependences of T_c and $\partial T_c/\partial \epsilon_F$ on ϵ_F are tabulated for two cases: in the BCS and Fröhlich models. A comparison is made between the calculated curves and the experimental data concerning the dependences of T_c and $\partial T_c/\partial P$ on the pressure P for rhenium. This yields the relative change of the density of states during the topological transition. The question of the effect of singularities in the density of the electron states on the tunneling characteristics of a superconductor is analyzed. The effect of a change in the topology of the Fermi surface on the temperature dependence of the coefficient of thermal expansion of a metal in its normal state is investigated. It is shown that, as $\epsilon_F \to \epsilon_c$ the linear dependence of the anomalous part of the thermal expansion coefficient on the temperature changes to a square root dependence.

1. INTRODUCTION

DURING measurements of the effect of the pressure P on the superconducting transition temperature T_c, a nonlinear dependence of T_c on P was observed in thalium in that range of pressures where the deformations are small.[1,2] Subsequent investigations of the combined effect of pressure and impurities of different valency on T_c indicated that the nonlinear dependence of T_c on P, and also the observed[3] maximum of the quantity $\partial T_c/\partial P$ as a function of the impurity concentration are related to the electronic properties of superconductors.[4,5] A theory constructed in[6] explains these experiments on the basis of the idea that the topology of the Fermi surface changes under the influence of impurities and pressure. As a result it became clear that these phenomena are not unique for thalium, but they should appear for all superconductors whose Fermi surface has a complicated structure with narrow necks or with small detached cavities. And in fact, as a result of subsequent experimental investigations, nonlinear dependences of the superconducting transition temperature and the maximum of its derivative with respect to pressure were observed for indium[4] and for rhenium.[7]

The present article is devoted to the further development of a theory of the manifestation of topological changes of the Fermi surface under the influence of external actions in the characteristics of a superconducting transition. We are primarily interested in the superconducting transition temperature. In this connection it will be shown how one can judge from the experimental data the nature of the topological transition and determine the relative change $\delta\nu/\nu$ in the density of states of the electrons, which is caused by this transition, and one can also determine the quantity $\partial(\epsilon_F - \epsilon_c)/\partial P$ where ϵ_F denotes the Fermi energy, and ϵ_c denotes the value of the electron energy at which the change in the topology of the equal-energy surfaces takes place.

The dependence of T_c and $\partial T_c/\partial \epsilon_F$ on ϵ_F is tabulated for two cases: in the BCS and Fröhlich models. A comparison is made between the calculated curves and the experimental data with regard to the dependences of T_c and $\partial T_c/\partial P$ on the pressure P for rhenium. Analysis of the experimental data indicates that for rhenium the quantity $\delta\nu/\nu$ is of the order of 10^{-2} for $\epsilon = \epsilon_c + 2T_c$, and the quantity $\partial(\epsilon_F - \epsilon_c)/\partial P$ is of the order of 10^{-4} eV/kbar. The question of the effect of singularities of the electron density of states on the tunneling characteristics of a superconductor is investigated. The influence of a change in the topology of the Fermi surface on the temperature dependence of the coefficient of thermal expansion of a metal in its normal state is studied. It is shown that, as $\epsilon_F \to \epsilon_c$ the linear dependence of the anomalous part of the coefficient of thermal expansion on the temperature is changed to a square-root dependence.

2. DEPENDENCE OF THE SUPERCONDUCTING TRANSITION TEMPERATURE ON THE FERMI ENERGY

If the Fermi energy is close to ϵ_c, then upon a small change of ϵ_F a change of the Fermi surface topology occurs, and the density of states $\nu(\epsilon_F)$ of the electrons on the Fermi surface has a singularity for $\epsilon_F = \epsilon_c$, so that one can represent $\nu(\epsilon)$ in the form of a sum of the smooth function $\nu_0(\epsilon)$ and a correction $\delta\nu(\epsilon)$ which contains a singularity at the point $\epsilon = \epsilon_c$:

$$\nu(\varepsilon) = \nu_0(\varepsilon) + \delta\nu(\varepsilon).$$

The singularity $\delta\nu(\epsilon)$ in the density of states appears in the dependence of T_c on ϵ_F (or on the parameters which change ϵ_F[1)]). In this section we consider the change of the superconducting transition temperature associated with a change in the Fermi energy of the electrons. We shall start from the equation which determines the energy gap C in a superconductor:[10]

[1)]We note that the Fermi energy of the electrons in a metal can be changed in such a way that it approaches ϵ_c, either with the aid of external pressure,[8] or else by the introduction of impurities.[9]

$$C(\mathbf{p}')=\frac{1}{2}\lambda^2\int J(\mathbf{p}',\mathbf{p})\frac{C(\mathbf{p})}{[\xi_p^2+C^2(\mathbf{p})]^{1/2}}\times\tanh\frac{[\xi_p^2+C^2(\mathbf{p})]^{1/2}}{2T}\frac{d\mathbf{p}}{(2\pi\hbar)^3},\qquad(2.0)$$

where λ is the coupling constant, ξ_p is the energy of the electrons measured from ϵ_F, T is the temperature, and $J(\mathbf{p}', \mathbf{p})$ is the kernel of the effective electron-electron attraction.[2)]

The expression for T_c, obtained from Eq. (2.0), in which the anisotropy of the electron-electron interaction is taken into account, differs from the expression for T_c with an isotropic electron-electron interaction by an amount δT_c which is proportional to

$$\delta T_c\propto\langle J^2(\mathbf{p}',\mathbf{p})\rangle-\langle J(\mathbf{p}',\mathbf{p})\rangle^2,$$

where $\langle\ldots\rangle$ denotes averaging over the directions of the vectors $\mathbf{p}'$ and $\mathbf{p}$. This difference is small even in that case when the anisotropy of $J(\mathbf{p}', \mathbf{p})$ amounts to 30%.[13] Therefore we shall assume for simplicity that the kernel $J(\mathbf{p}', \mathbf{p})$ depends only on the energy of the electrons, and we rewrite Eq. (2.0) in the form

$$C(\xi')=\frac{\lambda}{2V}\int_{-\epsilon_F}^{\infty}J(\xi',\xi)\nu(\varepsilon_F+\xi)\,\mathrm{th}\frac{[\xi^2+C^2(\xi)]^{1/2}}{2T}\frac{C(\xi)\,d\xi}{[\xi^2+C^2(\xi)]^{1/2}},\qquad(2.1)$$

where $\xi=\epsilon-\epsilon_F$ and V is the volume of the solid. For simplicity we shall assume that the kernel $J(\xi', \xi)$ of the effective electron-electron interaction does not have any singularities which are related to the change in the topology of the Fermi surface. This assumption agrees with the results of a calculation of $J(\xi', \xi)$ in the model of strongly bound electrons[14] (also see the end of Sec. 2 below).

Henceforth, following[15], it is convenient to change to the following dimensionless quantities:

$$\varphi(x,T)=\frac{C(\xi,T)}{C(0,T)},\quad K(x',x)=\frac{J(\xi',\xi)}{J(0,0)},\quad x=\frac{\xi}{\omega_D},$$

where ω_D denotes the Debye temperature, and Eq. (2.1) is rewritten in the form

$$\varphi(x')=\rho_0\int_0^{\infty}K(x',x)g(x)\,\mathrm{th}\frac{\{x^2+[\eta\varphi(x)]^2\}^{1/2}}{t}\frac{\varphi(x)\,dx}{\{x^2+[\eta\varphi(x)]^2\}^{1/2}}\qquad(2.2)$$

where

$$t=2T/\omega_D,\quad \rho_0=\lambda^2J(0,0)\nu_0(\varepsilon_F),$$

$$g(x)=\frac{\nu(\varepsilon_F+\omega_Dx)+\nu(\varepsilon_F-\omega_Dx)}{2\nu_0(\varepsilon_F)},\quad \eta=\frac{C(0,T)}{\omega_D}.$$

The quantity C(O, T) vanishes at the superconducting transition temperature $T = T_c$, and Eq. (2.2) takes the form

$$\varphi(x')=\rho_0\int_0^{\infty}K(x',x)g(x)\frac{\varphi(x)}{x}\,\mathrm{th}\frac{x}{t_\kappa}\,dx,\qquad(2.3)$$

where $t_c = 2T_c/\omega_D$. The superconducting transition temperature is determined from the equation

$$\frac{1}{\rho_0}=\int_0^{\infty}K(0,x)g(x)\frac{\varphi(x)}{x}\,\mathrm{th}\frac{x}{t_c}\,dx,\qquad(2.4)$$

which is obtained from expression (2.3) if one sets $x' = 0$ in it (according to definition $\varphi(0) = 1$).

Expressions (2.3) and (2.4) represent a system of equations for the determination of t_c and the gap $\varphi(x)$. In order to solve this system we shall utilize the smallness of the quantity t_c, and also the fact that the integrands have a singularity as $t_c \to 0$. By combining (2.3) with (2.4), multiplied by $-\rho_0K(x', 0)$, we obtain

$$\varphi(x')=K(x',0)+\rho_0\int_0^{\infty}[K(x',x)-K(x',0)K(0,x)]\times\varphi(x)g(x)\,\mathrm{th}\frac{x}{t_c}\frac{dx}{x}.\qquad(2.5)$$

One can solve Eq. (2.5) by the method of iterations, using the smallness of the parameter ρ_0, because now the integrand does not contain any singularity and one can set $t_c = 0$. In the zero-order approximation we have

$$\varphi(x)=K(x,0);$$

then Eq. (2.4) takes the form

$$\frac{1}{\rho_0}=\int_0^{\infty}|K(0,x)|^2g(x)\,\mathrm{th}\frac{x}{t_c}\frac{dx}{x}.\qquad(2.6)$$

Let us represent the normalized density g(x) of the electron-hole states in the form of a sum of two terms:

$$g(x)=g_0(x)+\delta g(x);$$

here

$$g_0(x)=[\nu_0(\varepsilon_F+\omega_Dx)+\nu_0(\varepsilon_F-\omega_Dx)]/2\nu_0(\varepsilon_F)$$

is a smooth function of ϵ_F, and

$$\delta g(x)=[\delta\nu(\varepsilon_F+\omega_Dx)+\delta\nu(\varepsilon_F-\omega_Dx)]/2\nu_0(\varepsilon_F)$$

contains the singularities resulting from the change in the topology of the equal-energy surface. Near the point ϵ_c one can write the correction $\delta\nu(\epsilon)$ in the form[16]

$$\delta\nu(\varepsilon)=\begin{cases}\mp a(\varepsilon_c-\varepsilon)^{1/2}\theta(\varepsilon_c-\varepsilon)\\ \mp a(\varepsilon-\varepsilon_c)^{1/2}\theta(\varepsilon-\varepsilon_c)\end{cases},\quad a=V\pi^{-2}K^*(2m_1m_2m_3)^{1/2},\qquad(2.7)$$

where the upper line pertains to that case when, upon an increase of the energy ϵ a transition occurs from a closed isoenergy surface to an open one (with the minus sign) or the disappearance of closed equal-energy surfaces (with the plus sign), and the lower line pertains to the case of the opposite transitions; m_1, m_2, m_3 denote the effective masses of the electron for $\epsilon = \epsilon_c$, and K^* is the number of equivalent points in the Brillouin zone corresponding to a given singularity.

Let us consider the change of T_c, due to the generation of a new cavity associated with the increase of the Fermi energy ($T_c = T_c^0 + \Delta T_c$). Then

$$\delta\nu(\varepsilon_F\mp\omega_Dx)=v(\beta+x/t_c^0)^{1/2}\nu_0(\varepsilon_F)\theta(t_c^0\beta+x),\quad v=\frac{a(2T_c^0)^{1/2}}{\nu_0(\varepsilon_F)},\quad \beta=\frac{\varepsilon_F-\varepsilon_c}{2T_c^0},\quad t_c^0=\frac{2T_c^0}{\omega_D}.\qquad(2.8)$$

The quantity $v \ll 1$ characterizes the relative change in the density of states near the Fermi surface, and the quantity β characterizes the distance from the Fermi surface to the critical point.

In that case when the singularities in the density of states are absent ($\delta g = 0$), Eq. (2.6) determines the dependence of T_c^0 on ϵ_F:

$$\frac{1}{\rho_0}=\int_0^{\infty}|K(0,x)|^2g_0(x)\,\mathrm{th}\frac{x}{t_c^0}\frac{dx}{x}.\qquad(2.9)$$

[2)] Equation (2.0) is valid in that case when one can neglect the damping of the quasiparticles.[11] Such a situation is realized for a number of superconductors (see[12]) including rhenium.

One can approximately solve Eq. (2.9) by using the smallness of the quantity t_c^0:[15]

$$\ln t_c^0 = -\frac{1}{\rho_0} - \int_0^\infty \frac{\ln x}{\mathrm{ch}^2 x} dx - \int_0^\infty \ln x \frac{d}{dx}[|K(0,x)|^2 g_0(x)]\,dx, \quad (2.10)$$

from which it follows that

$$T_c^0 = 2\gamma\pi^{-1}\chi\omega_D \exp(-1/\rho_0), \quad (2.11)$$

where $\ln\gamma$ is the Euler constant,

$$\ln\chi = -\int_0^\infty \ln x \frac{d}{dx}[K^2(0,x) g_0(x)]\,dx.$$

Usually in a discussion of the experimental data with regard to the superconducting transition temperature, one starts from the BCS formula:

$$T_c^0 = 2\gamma\pi^{-1}\omega_D \exp(-1/\rho_0) \approx 1.14\omega_D \exp(-1/\rho_0),$$

which corresponds to the kernel $K(0, x) = 1$ for $|x| \leq 1$ and $K(0, x) = 0$ for $|x| > 1$. At the same time it is clear that the value of the coefficient χ in the formula for T_c^0 depends on the form of the interaction kernel $K(0, x)$. In the Fröhlich-Debye model $K(0, x) = F(\omega_D x/2sk_F)$,[10,11] where

$$F(y) = 1 - 2|y| + 2y^2 \ln(1 + 1/|y|), \quad (2.12)$$

s is the speed of sound, and k_F is the Fermi momentum. In this case T_c^0 is determined by the formula

$$T_c^0 = 4\gamma A\pi^{-1} sk_F \exp(-1/\rho_0) \approx 0{,}44 sk_F \exp(-1/\rho_0), \quad (2.13)$$

where

$$\ln A = -\int_0^\infty \ln y \frac{d}{dy}[F(y)]^2\,dy \approx -1.64.$$

Now let us take the singularities in the density of states into account. In this case one can represent Eq. (2.6), with formulas (2.7), (2.8), and (2.10) taken into account, in the following form:

$$\ln\frac{t_c}{t_c^0} = \frac{v}{2}\int_{-t_\kappa^0\beta}^\infty |K(0,x)|^2 \left(\beta + \frac{x}{t_c^0}\right)^{1/2} \mathrm{th}\frac{x}{t_c}\frac{dx}{x}. \quad (2.14)$$

In the first-order approximation in the parameter v, we obtain the following expression for the relative change of the quantity T_c:

$$\Delta T_c / T_c^0 = {}^1/_2 v I(\beta), \quad (2.15)$$

where

$$I(\beta) = \int_{-\beta}^\infty |K(0, t_c^0 y)|^2 (\beta + y)^{1/2} \frac{\mathrm{th}\, y}{y} dy.$$

Expression (2.15) determines the nonlinear constituent in the dependence of T_c on ϵ_F. Qualitatively one can represent this dependence in the following manner:

$$\frac{\Delta T_c}{T_c^0} \approx \frac{1}{\rho_0}\frac{\delta\nu(\varepsilon_F)}{\nu_0(\varepsilon_F)} = \frac{v}{\rho_0}\left(\frac{\varepsilon_F - \varepsilon_c}{2T_c}\right)^{1/2}\theta(\varepsilon_F - \varepsilon_c). \quad (2.16)$$

Differentiating expression (2.15) with respect to the parameter β, we obtain

$$\frac{1}{T_c^0}\frac{\partial T_c}{\partial\beta} = \frac{v}{2}\frac{dI}{d\beta}. \quad (2.17)$$

Knowing the derivative $dT_c/d\beta$, it is not difficult to determine the derivative of T_c with respect to the pressure:

$$\frac{\partial T_c}{\partial P} = \frac{v}{4}\frac{\partial(\varepsilon_F - \varepsilon_c)}{\partial P}\frac{dI}{d\beta} \quad (2.18)$$

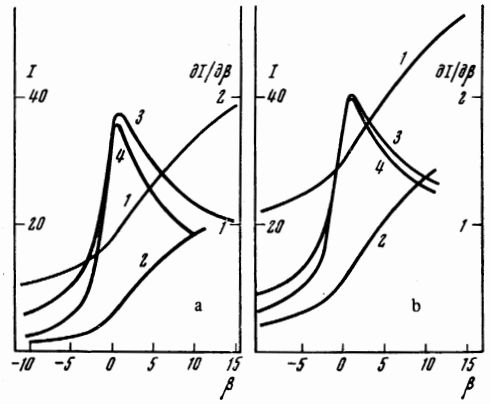

FIG. 1. The dependences of I on β (curves 1 and 2) and $dI/d\beta$ on β (curves 3 and 4): a–for the Fröhlich model with the following values of the parameters: curves 1, 3–$T_c/sk_F = 1/250$, curves 2, 4–$T_c/sk_F = 1/40$ and b–for the BCS model with the following values of the parameters: curves 1, 3–$2T_c/\omega_D = 1/250$, curves 2, 4–$2T_c/\omega_D = 1/40$.

Now let us present the integral $I(\beta)$ in explicit form for the following two cases: for the BCS model and for the Fröhlich-Debye model. In the first case

$$I(\beta) = \int_{-1/t_c^0}^{1/t_c^0} (\beta + y)^{1/2}\theta(\beta + y)\frac{\mathrm{th}\, y}{y} dy. \quad (2.19)$$

In the second case

$$I(\beta) = \int_{-\beta}^\infty F^2\left(\frac{T_c^0}{sk_F} y\right)(\beta + y)^{1/2}\frac{\mathrm{th}\, y}{y} dy, \quad (2.20)$$

where $F(x)$ is defined by formula (2.12). The results of a numerical calculation of the quantities $I(\beta)$ and $dI/d\beta$ are given in Fig. 1. As is evident from the figure, near the maximum the curves $dI/d\beta$ for the Fröhlich-Debye model are only slightly sensitive to the choice of the parameter T_c^0/sk_F; near the maximum the curves $dI/d\beta$ in the BCS model differ insignificantly from the curves in the Fröhlich-Debye model. These graphs determine the dependence of $\Delta T_c/T_c^0$ and dT_c/dP on the Fermi energy.

Formulas (2.15), (2.19), and (2.20) determine the dependence of ΔT_c on ϵ_F in that case when a new cavity of the Fermi surface is produced with an increase of ϵ_F. One can easily show that in the case of other topological transitions, the dependence of T_c^0 on ϵ_F is determined by these same integrals.

In addition to the nonlinear constituent of the dependence of the superconducting transition temperature on the pressure, which is due to the change in the topology of the Fermi surface, there also exists a linear component of the dependence of T_c on the pressure, $T_c^0(P) = T_c^0 + KP$, which is due to the small change of the superconductor's parameters under pressure. We shall also assume that the difference $\epsilon_F - \epsilon_c$ depends on the pressure linearly:

$$\beta(P) = z(P - P_c)/2T_c^0, \quad (2.21)$$

where $z = \partial(\epsilon_F - \epsilon_c)/\partial P$. Accordingly we represent the dependence of T_c on P in the form

$$T_c(P) = T_c^0 + KP + \frac{vT_c^0}{2}\begin{cases} \mp I(-z(P - P_c)/2T_c^0) \\ \mp I(z(P - P_c)/2T_c^0) \end{cases}. \quad (2.22)$$

Formula (2.22) describes four types of topological transitions in accordance with formula (2.7). The values

of the parameters K, v, z, P_c, and T_c^0 and the type of topological transition are determined from a comparison with experimental data.

In concluding this section let us analyze the equation of the effect of singularities in the density of states on the superconducting energy gap for $T \ll T_c$. Without dwelling on the calculations, which are analogous to those which were carried out in the calculation of T_c, we present the answer for the energy dependence of the gap:

$$C(\xi, \varepsilon_F - \varepsilon_c) = K\left(0, \frac{\xi}{\omega_D}\right) \Delta_0(\varepsilon_F)\,[1 + 0{,}47 v I_1(\beta_1)], \quad (2.23)$$

where $\xi = \epsilon - \epsilon_F$, $\Delta_0(\epsilon_F) = 1.76\, T_c^0$ denotes the value of the superconducting gap in the absence of singularities in the density of states, $\beta_1 = [\epsilon_F - \epsilon_c]/\Delta_0$, and

$$I_1(\beta_1) = \int_{-\beta_1}^{\infty} \left| K\left(0, \frac{\Delta_0}{\omega_D} x\right) \right|^2 \left(\frac{x + \beta_1}{1 + x^2}\right)^{1/2} dx. \quad (2.24)$$

The integral $I_1(\beta)$ essentially does not differ from the integral $I(\beta)$, because the functions $x^{-1}\tanh x$ and $(1 + x^2)^{-1/2}$ differ very slightly one from the other (compare formulas (2.24) and (2.15)).

From formula (2.23) it is seen that the expression for the gap corresponds to the product of the function $K(0, \xi/\omega_D)$, depending on the excitation energy ξ, times a function (standing inside the square brackets) which depends on the difference $\epsilon_F - \epsilon_c$. The dependence of the tunneling current on the stress is connected with the first factor, and the nonlinear dependence of the gap on the pressure is related to the second factor. Thus, the anomalies of the tunneling current are related to the form of the kernel $K(0, \xi/\omega_D)$. However, if $K(0, \xi/\omega_D)$ as a function of ξ were to have singularities related to the change in the topology of the Fermi surface, then this would lead to the appearance of asymmetric (with respect to a change in the sign of the applied stress) peaks in the derivatives of the tunneling current with respect to stress, in addition to the symmetric peaks associated with the singularities of the phonon spectrum. However, such asymmetric peaks have not yet been observed experimentally.[17] This fact justifies the assumption made earlier that the kernel $J(\xi', \xi)$ of the electron-electron interaction does not have any singularities which are related to the change in the topology of the Fermi surface.

3. DETERMINATION OF THE PARAMETERS THAT CHARACTERIZE A TOPOLOGICAL CHANGE OF THE FERMI SURFACE

As is evident from formulas (2.15)--(2.22) and Fig. 1, the experimentally observed nonlinear variation of T_c with pressure, correlated with the presence of a maximum (or minimum) of dT_c/dP, may be interpreted as the result of a change in the topology of the Fermi surface. One can find the parameters v, P_c, and z, characterizing this topological transition, from a comparison of the experimentally observed dependence $\Delta T_c(P) = T_c(P) - T_c(0)$ with the theoretical dependence, which is determined by the expression

$$\Delta T_c(P) = {}^1/_2 T_c^0 \tilde{v} I(\tilde{z}(P - P_c)/2T_c^0) - {}^1/_2 T_c^0 \tilde{v} I(-\tilde{z} P_c/2T_c^0) + KP, \quad (3.1)$$

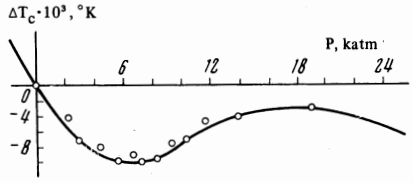

FIG. 2. Dependence of ΔT_c on P for rhenium: the curve represents the theoretical values, and the points correspond to the experimental data. [7]

where in conformity with formula (2.22) the following notation has been introduced: $\tilde{v} = \mp v$ and $\tilde{z} = \mp z$. If $\tilde{z} > 0$, then upon an increase of the pressure there occurs either the formation of new cavities of the Fermi surface (in the case $\tilde{v} > 0$) or the transition of an open Fermi surface into a closed one (for $\tilde{v} < 0$). However, if $\tilde{z} < 0$ then upon an increase of the pressure there occurs either the disappearance of the cavities of the Fermi surface ($\tilde{v} > 0$) or the transition of a closed Fermi surface into an open one ($\tilde{v} < 0$).

The result of a comparison between the experimental dependence of ΔT_c on P for rhenium with the theoretical dependence, determined by expression (3.1), is shown on Fig. 2. The values of the parameters $\tilde{v}$, $\tilde{z}$, P_c, and K were determined by the method of least squares:[3)]

$$\tilde{v} = 1.4 \cdot 10^{-2}, \quad \tilde{z} = 0.9 \cdot 10^{-4}\ \text{eV/katm},$$
$$K = -6.4 \cdot 10^{-3}\ \text{deg/katm}, \quad P_c = 6.6\ \text{katm}.$$

In view of the strong correlation between the values of the parameters $\tilde{v}$, $\tilde{z}$, and K in the range of pressures from 0 to 20 katm, their values are determined with large errors (~50%).

For a more accurate determination of the values of these parameters, it is necessary to know the experimental dependence of ΔT_c on P over a wider range of pressures. Such a dependence can be obtained by using the experimental data on $\Delta T_c(P)$ for rhenium containing impurities of osmium and tungsten (see Figs. 3 and 4). From Figs. 3 and 4 it is seen that the presence of osmium impurities shifts the curve $\Delta T_c(P)$ for pure rhenium toward the side of smaller pressures, but tungsten impurities shift it toward the side of larger pressures. Taking this data into account enables us to enlarge the range of effective pressures for the dependence $\Delta T_c(P)$.

Let us consider the change of the superconducting transition temperature under the influence of impurities and pressure. We shall assume that $\epsilon_F - \epsilon_c$ is a linear function of the impurity concentration c and of the pressure P:

$$\beta = \frac{z}{2T_c^0}(P - P_\kappa - \alpha c), \quad \alpha = -\frac{1}{z}\frac{\partial(\varepsilon_F - \varepsilon_c)}{\partial c}$$

Taking the influence of the impurities into account leads to the following generalization of formula (2.22):

$$T_c(P, c) = T_c^0(c) + KP + {}^1/_2 T_c^0 \tilde{v} I(\tilde{z}(P - P_\kappa - \alpha c)/2T_c^0). \quad (3.2)$$

Hence for the experimentally measurable difference $\Delta T_c(P, c) = T_c(P, c) - T_c(0, c)$ we have[4)]

[3)] In this connection it was assumed that for rhenium $T_c^0 = 1.7°K$, $k_F = 1.27 \times 10^8\ \text{cm}^{-1}$, $s = 0.47 \times 10^6$ cm/sec, and $T_c^0/sk_F = 1/250$.[18,19]

$$\Delta T_c(P, c) = {}^1/_2 T_c^0 \tilde{\nu} I(\tilde{z}(P - P_c - \alpha c)/2T_c^0) - {}^1/_2 T_c^0 \tilde{\nu} I(-\tilde{z}(P_c + \alpha c)/2T_c^0) + KP. \quad (3.3)$$

One can represent expression (3.3) in the following form:

$$\Delta T_c(P, c) = \Delta T_\kappa(P - \alpha c) - \Delta T_c(-\alpha c). \quad (3.4)$$

Thus, the function $\Delta T_c(P, c)$ of two variables is expressed in terms of a function $\Delta T_c(P^*)$ of a single variable, which is determined by expression (3.1), and moreover the argument P^* of this function may take both positive and negative values.

From formula (3.4) it is evident that the curves showing the dependence of ΔT_c on the pressure for different impurity concentrations (Figs. 3 and 4) represent isolated segments of the single curve $\Delta T_c(P^*)$ for pure rhenium, which are displaced along the pressure axis by an amount αc, and along the temperature axis by an amount $-\Delta T_c(-\alpha c)$. Analysis of the experimental data presented in Figs. 3 and 4 enables us to determine the quantity α for osmium and tungsten, and to more accurately determine the values of the parameters entering into formula (3.1). We find the following values:

$$\alpha_{Os} = -59 \pm 2.5 \text{ katm/at.\%}, \quad \alpha_W = 147 \pm 5 \text{ katm/at.\%},$$

$$\tilde{\nu} = (6 \pm 0{,}6) \cdot 10^{-3}, \quad P_\kappa = 7{,}4 \pm 0{,}05 \text{ katm},$$

$$K = (-4 \pm 0{,}1) \cdot 10^{-3} \text{ deg/katm} \quad \tilde{z} = (1{,}5 \pm 0{,}2) \cdot 10^{-4} \text{ ev eV/katm}.$$

The theoretical curve $\Delta T_c(P^*)$ corresponding to the found values of the parameters $\tilde{\nu}$, $\tilde{z}$, P_c, and K is depicted in Fig. 5. The points pertaining to the experimental data of Figs. 2–4 are also shown on this same figure.

From the results of the analysis of the experimental data it follows that $\tilde{\nu} > 0$ and $\tilde{z} > 0$. This permits one to conclude that for rhenium under the influence of pressure, a new cavity of the Fermi surface appears, which corresponds either to the formation of a new group of electrons ($z = \tilde{z}$) or else to the formation of a new group of holes ($z = -\tilde{z}$). Knowing the values of $\tilde{z}$ and P_c, one can easily determine the difference $\epsilon_F - \epsilon_c = -zP_c$ for pure rhenium, and also the values of the derivatives $\partial(\epsilon_F - \epsilon_c)/\partial c = z\alpha$ for osmium and tungsten impurities:

$$|\varepsilon_c - \varepsilon_c| = (11 \pm 2) \cdot 10^{-4} \text{ eV}$$

$$\left|\frac{\partial(\varepsilon_c - \varepsilon_c)}{\partial c_{Os}}\right| = (9 \pm 1) \cdot 10^{-3} \frac{\text{eV}}{\text{at.\%}},$$

$$\left|\frac{\partial(\varepsilon_c - \varepsilon_c)}{\partial c_W}\right| = (22 \pm 3) \cdot 10^{-3} \frac{\text{eV}}{\text{at.\%}}.$$

Differentiating expression (3.3) with respect to the pressure, one can determine the dependence of $dT_c/dP|_{P=0}$ on the impurity concentration:

$$dT_c/dP|_{P=0} = K + {}^1/_4 \tilde{\nu}\tilde{z} I'(-\tilde{z}(P_c + \alpha c)/2T_c^0). \quad (3.5)$$

[4]From formula (3.3) it follows that the dependence $T_c^0(c)$, due to all other mechanisms (decrease of the anisotropy of the gap, change in the Debye temperature, change in the density $\nu_0(\epsilon_F)$ of the electron states, etc.), which are not related to the change in the topology of the Fermi surface, do not enter into the experimentally measured quantity $\Delta T_c(P,c)$.

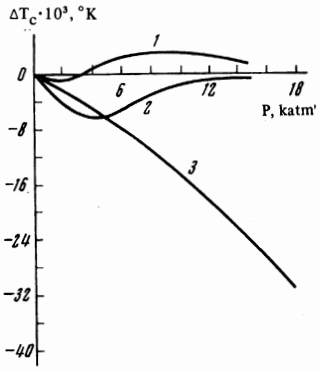

FIG. 3. Experimental dependence of ΔT_c on P for rhenium containing osmium impurities; [7] curve 1 is for Re + 0.05 at.% Os, curve 2 is for Re + 0.11 at.% Os, and curve 3 is for Re + 0.6 at.% Os.

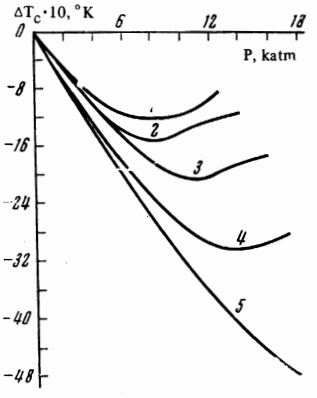

FIG. 4. Experimental dependence of ΔT_c on P for rhenium containing molybdenum and tungsten impurities: [7] curve 1 is for Re + 0.02 at.% Mo, curve 2 is for Re + 0.07 at.% Mo, curve 3 is for Re + 0.02 at.% W, curve 4 is for Re + 0.05 at.% W, and curve 5 is for Re + 0.1 at.% W.

The dependence of $dT_c/dP|_{P=0}$ on c for rhenium containing osmium impurities is shown in Fig. 6, the dependence being obtained by using the found values of the parameters.

Thus, the theory developed in the present article enables us to not only qualitatively but also quantitatively to describe the experimentally observed dependence of the superconducting transition temperature on the pressure and to determine from the experimental data such important characteristics as the change of the density of states associated with a topological transition, and also the value of the difference $\epsilon_F - \epsilon_c$.

4. THE EFFECT OF A CHANGE IN THE TOPOLOGY OF THE FERMI SURFACE ON THE PROPERTIES OF A METAL IN THE NORMAL STATE

The effect of singularities of the Fermi-surface topology on the thermodynamical properties of a metal in the normal state were investigated by I. Lifshitz[8] for the case $|\epsilon_c - \epsilon_F| \gg T$. In this section the tem-

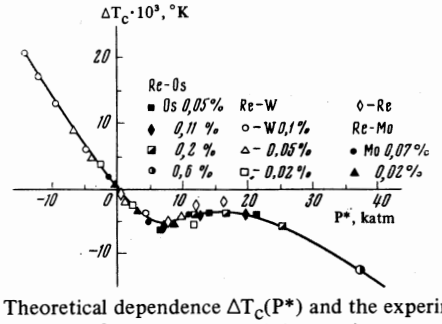

FIG. 5. Theoretical dependence $\Delta T_c(P^*)$ and the experimental data for pure rhenium and for rhenium containing osmium, tungsten, and molybdenum impurities.

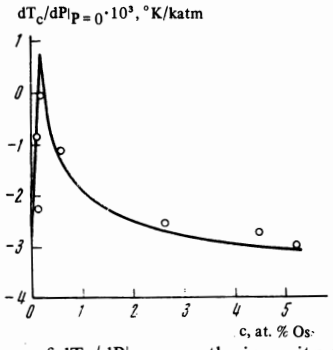

FIG. 6. Dependence of $dT_c/dP|_{P=0}$ on the impurity concentration of osmium in rhenium (theoretical curve and experimental data from [7]).

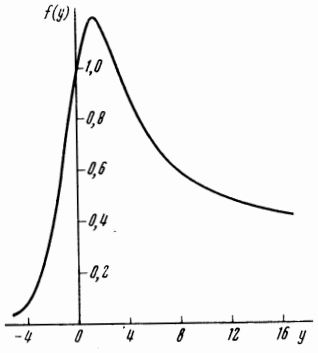

FIG. 7. The function f(y).

perature dependence of the coefficient of thermal expansion of the metal in the normal state is considered in that case when the Fermi energy is close to ϵ_c ($|\epsilon_c - \epsilon_F| \lesssim T$). As is well known, the coefficient of thermal expansion is given by

$$\alpha = V^{-1}(\partial V/\partial T)_P = V^{-1}\partial^2\Phi/\partial P\partial T = \alpha_0 + \delta\alpha, \qquad (4.1)$$

where α_0 and $\delta\alpha$ are respectively the normal and anomalous parts of the coefficient of thermal expansion. The anomalous part $\delta\Phi$ of the thermodynamic potential is determined by the formulas

$$\delta\Phi(T,P,N) = \delta\Omega(T,V,\mu) = -\int_0^\infty \frac{\delta N(\varepsilon)\,d\varepsilon}{e^{(\varepsilon-\mu)/T}+1}, \qquad (4.2)$$

where

$$\delta N = \int_0^\varepsilon \delta\nu(\varepsilon')\,d\varepsilon'$$

and $\delta\nu(\epsilon)$ is determined by formulas (2.7). From here one can easily find

$$\delta\alpha = \begin{cases} \pm aV^{-1}zT^{1/2}f((\varepsilon_c-\varepsilon_F)/T) \\ \pm aV^{-1}zT^{1/2}f((\varepsilon_F-\varepsilon_c)/T) \end{cases} \qquad (4.3)$$

where

$$f(y) = \frac{1}{2}\int_0^\infty \frac{3x-y}{e^{x-y}+1}\frac{dx}{\sqrt{x}}.$$

The function f(y), determining the dependence of $\delta\alpha$ on $(\epsilon_F - \epsilon_c)/T$, is shown in Fig. 7. From Fig. 7 and formulas (4.3) it is seen that, for Fermi energies close to ϵ_c, the anomalous part of the coefficient of thermal expansion significantly depends on ϵ_F, reaching an extremum for $|\epsilon_F - \epsilon_c|/T \approx 1.32$. If $\epsilon_F - \epsilon_c \gg T$, then[8]

$$\delta\alpha = \begin{cases} \pm\frac{\pi^2}{6}\frac{az}{V}\frac{T}{(\varepsilon_F-\varepsilon_c)^{1/2}} & \text{for } \varepsilon_F > \varepsilon_c \\ 0 & \text{for } \varepsilon_F < \varepsilon_c \end{cases} \qquad (4.4)$$

However, if $|\epsilon_F - \epsilon_c| \ll T$, then

$$\delta\alpha = \pm\frac{az}{V}f(0)T^{1/2} \approx \pm vz\frac{\nu_0(\varepsilon_F)}{V}\left(\frac{T}{2T_c}\right)^{1/2}. \qquad (4.5)$$

From these formulas it is clear that the temperature dependence of the anomalous part of the coefficient of thermal expansion changes substantially when the Fermi energy approaches the critical energy.

Since the dependence $\delta\alpha \propto T^{1/2}$ occurs for $\epsilon_F = \epsilon_c$, then at sufficiently low temperatures the anomalous part $\delta\alpha$ will play the major role in the coefficient of thermal expansion. In the case of negative values of $\delta\alpha$, a very unusual effect may be associated with this: At temperatures below a certain value, the metal will expand upon cooling. Let us present the dependence of $\delta\alpha$ on T for rhenium when $\epsilon_F = \epsilon_c$:[5)]

$$\delta\alpha = -44T^{1/2}\cdot 10^{-10}[1/°K]. \qquad (4.6)$$

The normal part of the coefficient of thermal expansion is given by[22]

$$\alpha_0 = (9T + 0{,}068T^3)\cdot 10^{-10}[1/°K]. \qquad (4.7)$$

Here the first and second terms describe, respectively, the electronic and lattice parts of the coefficient of thermal expansion. The temperature dependence of the coefficient of thermal expansion $\alpha = \alpha_0 + \delta\alpha$ for rhenium is shown in Fig. 8 for $\epsilon_F = \epsilon_c$. As is evident from Fig. 8 and from formulas (4.6) and (4.7), the contribution of the anomalous part $\delta\alpha$ becomes substantial at low temperatures, and the coefficient of thermal expansion changes sign at the temperature $T_0 \approx 9.4°K$.

The change in the temperature behavior of α can be observed experimentally if the condition $|\epsilon_F - \epsilon_c| < T_0$ is satisfied. Those metals for which the difference $\epsilon_F - \epsilon_c$ is sufficiently small, or else it can be made small with the aid of a small concentration of impurities, satisfy this condition. Thus, for rhenium, the required concentration of osmium impurities amounts to between 0.1 and 0.12 at.%.

In conclusion the authors thank A. I. Akhiezer, N. V. Zavaritskiĭ, and B. G. Lazarev for discussions of this work.

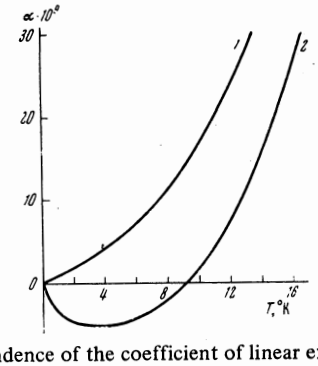

FIG. 8. Dependence of the coefficient of linear expansion on the temperature for rhenium: 1 is the experimental curve for pure rhenium, 2 is the theoretical curve for rhenium containing between 0.1 and 0.12 at. % of osmium impurities ($\epsilon_F \approx \epsilon_c$).

[5)]For calculations of the coefficient in formula (4.6) we utilized the value of the product $\bar{v}z$ found in the present work, and we assumed $\nu_0(\epsilon_F)/V = 6.6\times 10^{22}$ cm$^{-3}\cdot$eV^{-1} according to [20,21].

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Translated by H. H. Nickle
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