# *ANOMALIES IN THE SUPERCONDUCTING TRANSITION TEMPERATURE UNDER PRESSURE*

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It is shown that a change in the topology of the Fermi surface, induced in a superconductor by external pressure, leads to a nonlinear variation of the superconducting transition temperature $T_k$ with pressure. The relative change of $T_k$ is of the order of the square root of the ratio of the Debye frequency $\omega$ to the Fermi energy $\epsilon_0$.

1. The present experimental data on the effect of pressure on the superconducting transition temperature $T_k$ in various metals can be divided schematically into two groups. For most superconductors, a linear change of $T_k$ with pressure is observed. Thus, for example, for In, Cd and Pb, the value of $T_k$ decreases with increase in pressure, while for Ti and Zr, it increases. There is a different behavior of $T_k$ as a function of pressure for thallium. In the range of low pressures (up to 2000 atm), $T_k$ increases,[1] while upon a further increase in the pressure the superconducting transition temperature decreases.[2] In the region of "high" pressures, $T_k$ decreases according to a linear law, while the increase of $T_k$ in the region of "low" pressures has a nonlinear character.

The observed dependence of the superconducting transition temperature $\Delta T_k$ on pressure for Tl can be expressed as the sum of two components, one of which decreases according to a linear law with increase in pressure and the other increases nonlinearly in the region of low pressures, and approaches a constant value at high pressures.[3] The hypothesis has been advanced[3,4] that the nonlinear part of the dependence of $T_k$ on the pressure can be connected with a change in the topology of the Fermi surface under pressure. This hypothesis does not contradict the investigations of the concomitant effect on the superconducting transition temperature of impurities and pressure.[5,6] In this case, it was shown that the maximum of the derivative $dT_k/dP$ as a function of pressure is associated with the nonlinear component of $\Delta T_k(P)$.[6]

By starting out from the simplest model of superconductivity,[7,8] it is shown in the present work that one of the reasons for the nonlinear dependence of $\Delta T_k$ on the pressure can be a change in the topology of the Fermi surface under pressure. Since the change in the topology of the Fermi surface is associated with a change in the Fermi energy $\epsilon_0$ with pressure, we shall in what follows compute the variation of the superconducting transition temperature with variation of $\epsilon_0$. If a closed Fermi surface transforms to an open one with increase in $\epsilon_0$, or a new cavity is formed, then the superconducting transition temperature increases. If on the other hand an open Fermi surface transforms to a closed one, or one of the cavities disappears, then $T_k$ decreases.[1)]

It is shown that the contribution to $\Delta T_k(\epsilon_0)$ from this mechanism has a nonlinear character and is especially large for a variation of $\epsilon_0$ from $\epsilon_k - \omega$ to $\epsilon_k + \omega$, where $\epsilon_k$ is the value of the energy of the conduction electrons for which the character of the surface $\epsilon(p) = \epsilon$ changes; $\omega$ is the Debye frequency. If $\epsilon_0 < \epsilon_k - \omega$ or $\epsilon_0 > \epsilon_k + \omega$, then upon further increase in $\epsilon_0$ the contribution to $\Delta T_k$ from this mechanism tends to a certain constant value. The relative variation of $T_k$ in this case is equal to $\delta T_k/T_k \sim (\omega/\epsilon_0)^{1/2}$ in order of magnitude, the derivative $dT_k/d\epsilon_0$ has a maximum for $\epsilon_0 = \epsilon_k$. The specific character of the change in the topology of the Fermi surface can be discussed in terms of the asymmetry of the derivative $dT_k/d\epsilon_0$ as a function of $\epsilon_0$ relative to the maximum point $\epsilon_0 = \epsilon_k$.

2. The singularities in the density of electron states per unit energy range $\nu(\epsilon)$ and their effect on the thermodynamic characteristics of the metal in the normal state were considered by I. Lifshitz.[9] In order to take into account the effect of the

[1)]It can be supposed that the decrease of $T_k$ with pressure in tin[3] is explained by one of these transitions.

singularities of $\nu(\epsilon)$ on the thermodynamic properties of the metal in the superconducting state, we shall begin with the simplest model of the superconductor.

The equation which defines the dependence of the gap $\Delta$ in the energy spectrum on the temperature T has in this case the form

$$1=\frac{\lambda}{2}\int\limits_{-\omega}^{\omega}\frac{\operatorname{th}(\sqrt{\xi^2+\Delta^2(T)}/2T)}{\sqrt{\xi^2+\Delta^2(T)}}\nu(\varepsilon_0+\xi)\,d\xi, \qquad (1)^*$$

where $\lambda$ is the constant of electron-electron interaction and

$$\nu(\varepsilon)=\frac{1}{(2\pi)^3}\int\limits_{\varepsilon}\frac{dS}{v}.$$

Near those values of the energy $\epsilon_0$ where the character of the topology of the Fermi surface changes, $\nu(\epsilon)$ can be written in the form

$$\nu(\varepsilon)=\nu_0(\varepsilon)+\delta\nu(\varepsilon), \qquad (2)$$

where $\nu_0(\epsilon)$ is a smooth function of the energy, and $\delta\nu(\epsilon)$ is equal to[9]

$$\delta\nu(\varepsilon)=\begin{cases}\mp {}^1\!/_2 m_1\pi^{-2}[2m_3(\varepsilon_k-\varepsilon)]^{1/2}\,\theta(\varepsilon_k-\varepsilon),\\ \mp {}^1\!/_2 m_1\pi^{-2}[2m_3(\varepsilon-\varepsilon_k)]^{1/2}\,\theta(\varepsilon-\varepsilon_k).\end{cases} \qquad (2')$$

The upper sign on the right hand side of Eq. (2′) refers to the case of a transition from a closed Fermi surface to an open one (with minus sign) or the disappearance of one of the cavities of the Fermi surface (with plus sign), the lower sign refers to the case of reverse transitions; $m_1$, $m_3$ are the effective masses of the electron at $\epsilon=\epsilon_k$; $\theta(x)=1$ if $x>0$ and $\theta(x)=0$ if $x<0$.

Let us consider the variation of the gap $\Delta$, $T_k$, and $H_k$ brought about by transitions from a closed Fermi surface to an open one. The analysis of the remaining cases is similar and we shall not present it here. Substituting $T=0$ in (1) and carrying out integration in the usual way with the smooth part of the density of the electron states $\nu_0(\epsilon)$, we get an equation for the gap $\Delta$:

$$\lambda\nu_0(\varepsilon_0)\ln\frac{2\omega}{\Delta_0}=1+\frac{\lambda m_1(2m_3)^{1/2}}{2\pi^2}\int\limits_{-\omega}^{\omega}\frac{(\varepsilon_k-\varepsilon_0-\xi)^{1/2}}{(\xi^2+\Delta_0^2)^{1/2}}\times\theta(\varepsilon_k-\varepsilon_0-\xi)\,d\xi. \qquad (3)$$

Assuming $|\epsilon_k-\epsilon_0|\ll\epsilon_0$, we then find

$$\frac{1}{\Delta_0}\frac{d\Delta_0}{d\varepsilon_0}\sim\frac{m_1(2m_3)^{1/2}}{2\pi^2\nu_0(\varepsilon_0)}\int\limits_{-\omega}^{\omega}\frac{\theta(\varepsilon_k-\varepsilon_0-\xi)\,d\xi}{[(\xi^2+\Delta^2)(\varepsilon_k-\varepsilon_0-\xi)]^{1/2}}. \qquad (4)$$

As is seen from Eq. (4), the size of the gap increases with increase in energy, while the derivative $d\Delta_0/d\epsilon_0$ approaches its largest value for $\epsilon_1=\epsilon_k$ and is equal to

$$\left(\frac{d\Delta_0}{d\varepsilon_0}\right)_{\varepsilon_0=\varepsilon_k}\approx 1.85\frac{m_1(2m_3)^{1/2}\Delta_0^{1/2}}{\pi^2\nu_0(\varepsilon_0)}=1.85\frac{|\delta\nu(\varepsilon_0-\Delta_0)|}{\nu_0(\varepsilon_0)}. \qquad (5)$$

Schematically, the dependence of $d\Delta_0/d\epsilon_0$ on $\epsilon_0$ in the case of the simplest topological variations of the Fermi surface is shown in Fig. 1.

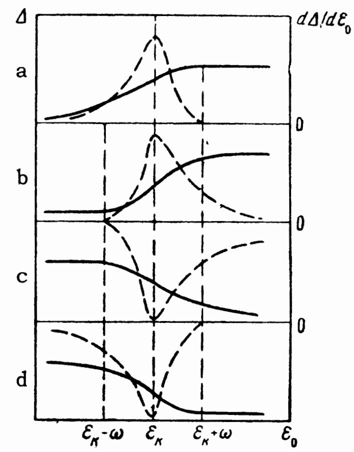


FIG. 1. Dependence of $\Delta$ (solid line) and $d\Delta/d\epsilon_0$ (broken line) on $\epsilon_0$ following a change in the topology of the Fermi surface: a – transition of a closed Fermi surface to an open one ($d\Delta/d\epsilon_0>0$), b – formation of a new cavity in the Fermi surface ($d\Delta/d\epsilon_0>0$), c – transition of an open Fermi surface to a closed one ($d\Delta/d\epsilon_0<0$), d – disappearance of one of the cavities of the Fermi surface ($d\Delta/d\epsilon_0<0$).

The solution of Eq. (3) with respect to $\Delta_0$ has in general a complicated form. We shall write it out for several limiting cases. The largest value of the gap size is reached for $\epsilon_0=\epsilon_k+\omega$, and is equal to

$$\Delta=2\omega\exp\{-1/\lambda\nu_0(\varepsilon_0)\}. \qquad (6)$$

If $\epsilon_0=\epsilon_k$, then

$$\Delta=2\omega\exp\{-1/\lambda\nu_0(\varepsilon_0)+\delta\nu(\varepsilon_0-\omega)/\nu_0(\varepsilon_0)\} \qquad (6')$$

and, finally, for $\epsilon_0\le\epsilon_k-\omega$,

$$\Delta=2\omega\exp\{-1/\lambda\nu(\varepsilon_0)\}. \qquad (6'')$$

Schematically, the dependence of the gap on $\epsilon_0$ is also shown in Fig. 1. It should be noted that the relative correction to the value of the gap in the energy interval $\epsilon_k-\omega\le\epsilon_0\le\epsilon_k+\omega$ brought about by the change in the topology of the Fermi surface is of the order of $(\omega/\epsilon_0)^{1/2}$ while the correction to the gap brought about by dependence on the energy of the coupling constant $\lambda$ and the quantity $\nu_0(\epsilon)$ is generally of the order $\omega/\epsilon_0$, that is, significantly smaller.

3. Starting out from Eq. (1), one can determine

*th ≡ tanh.

the variation on the superconducting transition temperature $T_k$ with variation of the Fermi energy $\epsilon_0$. This change, together with the change in the gap, is especially large in the range of values of $\epsilon_0$ from $\epsilon_k - \omega$ to $\epsilon_k + \omega$. Setting $T = T_k$, $\Delta(T_k) = 0$, we rewrite Eq. (1) in the form

$$1 = \frac{\lambda}{2}\int_{-\omega}^{\omega} \frac{\operatorname{th}(|\xi|/2T_k)}{|\xi|} \nu(\varepsilon_0+\xi)\,d\xi. \qquad (7)$$

Using Eqs. (2) and (2′) and taking the continuous function $\nu_0(\epsilon_0)$ outside the integral sign, we get

$$\lambda\nu_0(\varepsilon_0)\ln\frac{\omega\gamma}{\pi T_k} = 1 + \frac{\lambda m_1(2m_3)^{1/2}}{2\pi^2} \times \int_{-\omega}^{\omega} \frac{\operatorname{th}(|\xi|/2T_k)(\varepsilon_k-\varepsilon_0-\xi)^{1/2}}{|\xi|}\theta(\varepsilon_k-\varepsilon_0-\xi)\,d\xi, \qquad (8)$$

where $\ln\gamma = C = 0.577$.

Differentiating this equation with respect with $\epsilon_0$, it is not difficult to establish the fact that for $\epsilon_k - \omega \le \epsilon_0 \le \epsilon_k + \omega$, the derivative of $T_k$ with respect to $\epsilon_0$ is positive (that is, $T_k$ increases with increase in $\epsilon_0$) and reaches its largest value at $\epsilon_0 = \epsilon_k$ equal to

$$\left(\frac{dT_k}{d\varepsilon_0}\right)_{\varepsilon_0=\varepsilon_k} \approx 1.4\left|\frac{\delta\nu(\varepsilon_0-T_k)}{\nu_0(\varepsilon_0)}\right|. \qquad (9)$$

The dependence of $dT_k/d\epsilon_0$ on $\epsilon_0$ is similar to the dependence of $d\Delta_0/d\epsilon_0$ on $\epsilon_0$.

The largest value of $T_k$ is achieved for $\epsilon_0 = \epsilon_k + \omega$:

$$T_k = \frac{\gamma\omega}{\pi}\exp\left\{-\frac{1}{\lambda\nu_0(\varepsilon_0)}\right\}. \qquad (10)$$

If $\epsilon_0 = \epsilon_k$, then the superconducting transition temperature is equal to

$$T_k = \frac{\gamma\omega}{\pi}\exp\left\{-\frac{1}{\lambda\nu_0(\varepsilon_0)} + \frac{\delta\nu(\varepsilon_0-\omega)}{\nu_0(\varepsilon_0)}\right\}, \qquad (11)$$

and, finally, for $\epsilon_0 < \epsilon_k - \omega$ the value of $T_k$ takes on the value

$$T_k \approx \frac{\gamma\omega}{\pi}\exp\left\{-\frac{1}{\lambda\nu(\varepsilon_0)}\right\}. \qquad (12)$$

4. The singularities of the state density brought about by the change in the topology of the Fermi surface also give information on the value of the critical magnetic field $H_k$. In order to estimate this effect, we compare the difference between the free energy F in the normal and superconducting state with the magnetic energy density. The difference $F_s - F_n$ is equal to [8]

$$F_s - F_n = \int_0^{\Delta(T)} \frac{d}{d\Delta}\left(\frac{1}{\lambda}\right)\Delta^2 d\Delta = -\frac{H_k^2}{8\pi}.$$

Using Eq. (1), we get

$$\frac{H_k^2}{8\pi} = -\frac{1}{2}\int_{-\omega}^{\omega}\nu(\varepsilon_0+\xi)\,d\xi \int_0^{\Delta(T,\varepsilon_0)} \frac{d}{dz}\left\{\frac{\operatorname{th}[(\xi^2+z^2)^{1/2}/2T]}{(\xi^2+z^2)^{1/2}}\right\}z^2dz.$$

Since both quantities $\nu(\epsilon_0)$ and $\Delta(T, \epsilon_0)$ increase with increase in $\epsilon_0$ in the transition from a closed Fermi surface to an open one (or in the appearance of a new cavity), $H_k^2/8\pi$ also increases in this case, i.e., $dH_k/d\epsilon_0 > 0$. The maximum value of the quantity $H_k^2$ is achieved for $\epsilon_0 = \epsilon_k + \omega$ and the formulas for $H_k$ in this case have the usual form.[8]

The derivative of $H_k$ with respect to $\epsilon_0$ is a maximum as also are $d\Delta_0/d\epsilon_0$, $dT_k/d\epsilon_0$ for $\epsilon_0 = \epsilon_k$. If $\epsilon_0 = \epsilon_k$, then $H_k^2$, in the region of temperatures much less than in the superconducting transition temperature, is determined by the equation

$$H_k^2/8\pi \approx {}^1\!/_2\Delta^2[\nu_0(\varepsilon_0) + 0.2\delta\nu(\varepsilon_0-\Delta)] + {}^2\!/_3\pi^2\nu_0(\varepsilon_0)T^2, \qquad (13)$$

where $\Delta$ is determined by Eq. (6′). Thus, the contributions to $H_k^2$ are of the order of $(\Delta/\epsilon_0)^{1/2}$ in comparison with the usual formulas and the smooth change of $H_k$ brought about by the change in $\Delta$. For a temperature that is sufficiently close to $T_k$, the value of $H_k$ is proportional to $1 - T/T_k$. However, the constant of proportionality decreases relative to the usual expression by an amount of the order of $(\omega/\epsilon_0)^{1/2}$.

5. Since the density of electrons in the metal changes with change in the external pressure, and consequently the Fermi energy also changes, then in the region of pressures P close to $P_k$, which corresponds to a Fermi energy $\epsilon_0$ close to $\epsilon_k$, a nonlinear change of the thermodynamic characteristics of the superconductor with pressure ($T_k$, $H_k$ and $\Delta$) should be observed. To study the specific character of the variation of the topology of the Fermi surface, it is necessary to study the derivative $dT_k/dP$ with great accuracy and detail. The introduction of impurities can make it possible to observe the nonlinear change of $T_k$ in a region of comparatively low pressures.

Experiments on the effect of pressure on $T_k$ in thallium (Fig. 2, curve 1), [6] can be interpreted in the following fashion, on the basis of what has been set forth above. In the case of pure thallium, the energy $\epsilon_0$ is somewhat higher than $\epsilon_k$, but the difference $\epsilon_0 - \epsilon_k$ is less than $\omega$ (Fig. 1b). This leads to the result that in the region of low pressures, the nonlinear component, with which the increase of $T_k$ is associated, predominates (see Fig. 2, curve 1). Upon increase in pressure, the nonlinear contribution to $\Delta T_k$ reaches some constant value and the increase in $T_k$ according to the

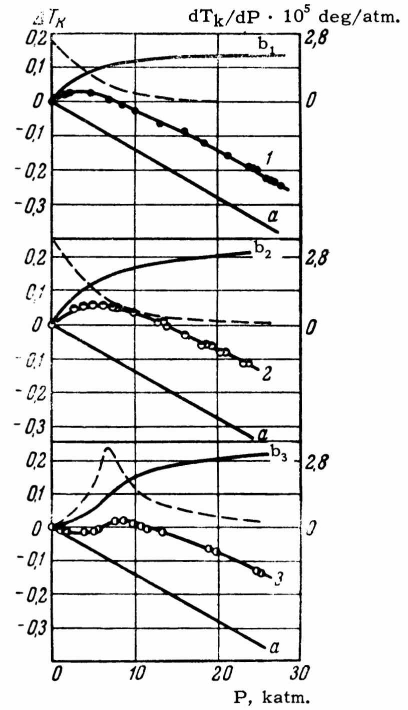


FIG. 2. Dependence of the change of superconducting transition temperature in thallium and its alloys on the pressure;[6] curve I – pure Tl, 2 – Tl-Hg (0.45 at. % Hg); 3 – Tl - Hg (0.9 at. % Hg); curve a – linear component, $b_1$, $b_2$, $b_3$ – nonlinear components of curves 1, 2, 3, respectively. The dashed lines are the nonlinear parts of the dependence of $dT_k/dP$ on the pressure.

linear law at high pressures is connected with the dependence on pressure of $\omega$, $\nu_0$, and $\lambda$.

The addition of impurities leads to a decrease in $\epsilon_0$. Two cases are possible: if the valence of the impurity is larger than the valence of thallium, then the difference $\epsilon_0 - \epsilon_k$ increases, and the role of nonlinear contribution in $\Delta T_k(P)$ decreases (Fig. 1b). If the valence of the impurity is lower than that of thallium, then the difference $\epsilon_0 - \epsilon_k$ decreases, which leads to an increase in the role of nonlinearity of the contribution to the increase in the maximum on the curve $\Delta T_k(P)$ for not too high a concentration of impurities (0.45 at% Hg; see Fig. 2, curve 2).

Upon further increase in the impurity concentration, when $\epsilon_0 < \epsilon_k - \omega$ (Fig. 1b) in the region of low pressures, $\Delta T_k$ decreases with pressure as the result of the linear component. Under the effect of the pressure, $\epsilon_0$ increases and in the region $\epsilon_k + \omega > \epsilon_0 > \epsilon_k - \omega$ the nonlinear component in $\Delta T_k(P)$, associated with the change in topology of the Fermi surface (see Fig. 2, curve 3), becomes dominant. With further increase in the pressure (and $\epsilon_0$), the linear component in $\Delta T_k(P)$ again plays the dominant role, since the nonlinear component reaches its limiting value. Such a behavior of $\Delta T_k$ with pressure was observed in Tl - Hg 0.9 at% (see Fig. 2).

By the asymmetry of the dependence of $dT_k/dP$ on P (Fig. 2), which is brought about by the nonlinear component, thallium can be associated with the case b of Fig. 1. The presence in thallium of a Fermi surface with $\epsilon_0 - \epsilon_k \sim \omega$ does not contradict the experimental data on the de Haas–Van Alphen effects[10] and the absorption of ultrasound in the magnetic field.[11]

We note that anisotropy of the gap and of the lattice has not been considered by us; however, in our opinion this would not qualitatively change the results.

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