ANOMALOUS PROPERTIES OF SUPERCONDUCTING COMPOUNDS OF THE V_3Si TYPE

E. I. KATS

Institute of Theoretical Physics, USSR Academy of Sciences

Submitted February 12, 1968

Zh. Eksp. Teor. Fiz. 55, 584–588 (July, 1968)

The behavior of compounds of the V_3Si type at low temperature is considered by starting from the energy-band model[1]. The effect of a magnetic field on the properties of these compounds is investigated. The results agree qualitatively with the experimental data[2].

1. Labbe and Friedel[3] considered in the energy-band model[1] the low-temperature properties of compounds of the V_3Si type. They have shown that at sufficiently low temperatures (below a certain value T_m) such compounds are unstable against martensitic transformation of the cubic phase into the tetragonal phase. They interpreted such a transformation as an effect connected with the instability of the electronic spectrum of the cubic phase, due to the presence of a peak in the density of states near the boundary of the narrowest of the three d-bands. In a subsequent paper[4] they explained in the same manner the singularities of the superconducting transition in these compounds. At temperatures $T < T_c < T_m$, the effective BCS interaction is realized in a very narrow energy region near the maximum of the state density. The width of this peak is much smaller than the Debye frequency. This yields, for example, a quadratic dependence of the gap on the interaction, the absence of an isotopic effect, and many other deviations from the usual BCS theory. However, these two transitions were considered separately, whereas it will be shown subsequently that these two phenomena are interrelated and must be investigated jointly. The same interaction which leads to a pairing of the d-electrons is also responsible for the structure phase transition. The gist of the effect is that the following process can occur in compounds of this group, in which the flat d-band comes sufficiently close to the s-band: in the presence of an effective attraction in the d-band, it is more convenient for the s-band electrons to go over into the d-band and produce there a bound state. Therefore the number of electrons in the d-band is anomalously small (on the order of the number of pairs), and all are paired. Thus, the proposed mechanism is strongly influenced by the closeness of the d- and s-bands ($\sim 10°K$) and by the quasi-one-dimensional character of the d-electron motion: $m_\perp \gg m_\parallel$ ($m_\perp$, $m_\parallel$—transverse and longitudinal effective masses).

2. In the tight-binding approximation, the Fermi surface of the electron constitutes three mutually-perpendicular flat layers. In the case of sufficiently thin layers, corresponding to $Q \ll 1$ electrons per transition-element atom (according to the estimates of Labbe and Friedel, the real value of Q for V_3Si is ~ 0.05), the contribution from the Cooper diagram (Fig. 1) will be

$$K_1 = \begin{cases} gm^{1/2}T^{-1/2}, & \mu/T \ll 1 \\ gm^{1/2}\mu^{-1/2}, & \mu/T \gg 1 \end{cases} \quad (1)$$

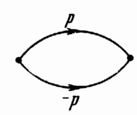

FIG. 1.

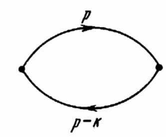

FIG. 2.

Here g—constant of effective electron-electron interaction and μ—chemical potential. This gives a singularity in the vertex function at $T \sim T_c \sim g^2m$. However, under the same assumptions, the zero-sound contribution at momentum transfers $k \sim 2p_0$ (Fig. 2) is of the same order of magnitude

$$N_1 = \begin{cases} -g_1m^{1/2}T^{-1/2}, & \mu/T \ll 1 \\ -g_1m^{1/2}\mu^{-1/2}e^{2\mu/T}, & \mu/T \gg 1, \end{cases} \quad (2)$$

g_1—interaction constant at momentum transfers $\sim 2p_0$. Therefore, both types of contributions should be studied jointly. However, the situation here is not of the "parquet" type[5], since, for example, the contribution of the diagram of the "envelope" type (Fig. 3) has the same order $g^3m^{3/2}T_c^{-3/2}$ at $\mu/T_c \ll 1$. Physically this is connected with the fact that processes with arbitrary number of particles have an anomalously large value. Consequently, it is impossible to separate in this problem the principal "most diverging" diagrams. Nonetheless, qualitative conclusions can be drawn concerning the properties of such systems.

3. To consider the elastic properties, we write out the phonon Green's function

$$D^{-1} = D_0^{-1} - N. \quad (3)$$

Here D_0—Green's function of the non-interacting phonons. It follows from (3) and (2) that at a temperature $\sim T_m \sim g_1^2m$ a possibility arises for sound to propagate in the system with anomalously low velocity, i.e., the corresponding elastic moduli vanish. This corresponds to instability against martensitic transformation in such systems. The elastic moduli actually do not

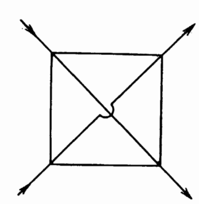

FIG. 3.

vanish, but decrease to a certain value, followed by a first-order phase transition with a small jump. It follows from the experimental data[2] that $T_m > T_c$ and consequently $g_1 > g$, which may be evidence in favor of the non-phonon mechanism of the effective attraction. From the symmetry of the Fermi surface it is easy to see that with anomalously low velocity, transverse phonons enter into expression (3). The components of the deformation potential for the longitudinal and transverse phonons are related in order of magnitude like $b^2/p_0^2 \ll 1$, where b—thickness of the "Fermi layer," and p_0—Fermi momentum. This agrees with the anomalous decrease, at $T \sim T_m$, of just the transverse elastic moduli $(c_{11} - c_{22})$. This fact can be related in turn with the rapid growth of the sound absorption coefficient near T_c (since the absorption coefficient $a_s \sim v_s^{-3}$, where v_s is the speed of sound). This result agrees with the conclusions of Labbe and Friedel. However, as seen from the foregoing, it has only a qualitative character.

4. As indicated above, the same interaction leads to the possibility of "pairing" of the d-band electrons. However, the nature of the effect is much more complicated, since the diagrams corresponding to the interaction of an arbitrary number of electrons also have anomalous values. This is connected with the absence of the gas approximation in the one-dimensional case. On the other hand, if we confine ourselves for a qualitative consideration only to the Cooper pairing, then, as usual, it is necessary to introduce the function

$$F = \frac{\Delta}{\omega^2 - \varepsilon^2(p) - |\Delta|^2}, \tag{4}$$

where Δ is the gap. From this we get an equation for the gap

$$1 = gm^{1/2}/\sqrt{\Delta}. \tag{5}$$

It should be noted once more that these formulas have a qualitative character, and for an exact solution of the problem it would be necessary to sum the entire sequence of diagrams. A result similar to (5) was obtained also in[4]. Yet, the authors of the latter paper claim an exact quantitative meaning for this formula (they calculate T_c); this, as seen from the foregoing, is not valid. In addition, no account was taken in[4] of the possible influence of pairing in the s-band, which can change the results.

5. To take the s-d interaction into account, we write down the simultaneous system of equations for the gaps. If we taken into account everything said above concerning formula (5), we can write (retaining only K_i)

$$\Delta_s = -g_s\Delta_s m_s p_0 \ln\frac{\tilde{\omega}}{\Delta_s} - \lambda_{sd}\sqrt{m_d}\,\Delta_d^{1/2},$$
$$\Delta_d = -\lambda_{sd}\Delta_s m_s p_0 \ln\frac{\tilde{\omega}}{\Delta_s} - g_d\sqrt{m_d}\,\Delta_d^{1/2}. \tag{6}$$

The indices s and d denote here the s and d bands, $\tilde{\omega}$—characteristic cut off energy (for example, the Debye frequency in the phonon mechanism of attraction), and λ_{sd}—effective interaction. Solution of the system (6), for example in the case when

$$\Delta_s g_s m_s p_0 \ln(\tilde{\omega}/\Delta_s) \ll \lambda_{sd}\sqrt{m_d}\Delta_d^{1/2}, \tag{7}$$

yields the following expressions for the gaps:

$$|\Delta_d| = \lambda_{sd}^4 m_s^2 p_0^2 m_d \ln^2\frac{\tilde{\omega}}{\lambda_{sd}^3 m_s p_0 m_d}, \tag{8}$$
$$|\Delta_s| = \lambda_{sd}^3 m_s p_0 m_d \ln\frac{\tilde{\omega}}{\lambda_{sd}^3 m_s p_0 m_d}$$

Formulas (8) replace in the "two-band model" expression (5) for the gap. Another possible influence of the s-band corresponds to allowance for the processes of the scattering of the d-pair against the Fermi background of the s-band. This causes renormalization of the chemical potential and "smearing" of the level corresponding to the bound state, on the order of $g_d\lambda_{sd}^2 m_s^2 p_0 \ln(\tilde{\omega}/\omega)$.

Allowance for the s-band makes it also possible to determine conveniently the value of the chemical potential from the condition for the conservation of the total number of particles.

6. We can also consider qualitatively the electromagnetic properties of such superconductors. The singularities in the temperature dependence of the paramagnetic susceptibility and of the Knight shift in the normal state were recently investigated by Labbe[6]. We shall consider, on the other hand, the superconducting state in a constant magnetic field. Since the Fermi surface of the d-band is flat, current will not flow in this band

$$j_d = 0, \tag{9}$$

and in the s-band we obtain the usual expression for the current

$$j_s = -\frac{n_s e^2}{m_s} Q_s(\mathbf{k})\mathbf{A}, \tag{10}$$

where Q_s—integral kernel.

An interesting phenomenon takes place when the field is increased. Since the field does not act on the one-dimensional d-gap, owing to gauge invariance, and since the system (6) has no solutions with $\Delta_s = 0$ but $\Delta_d = 0$, for λ_{sd} we can propose several mechanisms for the destruction of the superconductivity. Thermodynamic destruction corresponds to a critical field at $T = 0°K$

$$H_c^2(0)/8\pi = \tfrac{1}{2}N_d\Delta_d^2 + \tfrac{1}{2}N_s\Delta_s^2, \tag{11}$$

where N_d and N_s are the state densities in the corresponding bands.

In strong fields, the phases of three d-gaps can add up in such a way that the total d-gap vanishes. Then, since Eqs. (6) lead to

$$|\Delta_s| \sim \lambda_{sd}\sqrt{m_d}\Delta_d^{1/2},$$

it follows that $eH_{c1} \sim \Delta_s^2 v_s^{-2}$, where v_s is the Fermi velocity in the S-band. In fields $H \lesssim H_{c1}$ we then get $j_d = 0$, while j_s and Δ_s satisfy an equation of the Landau-Ginzburg type. If the phases were to combine in this manner, an appreciable nonlinearity of the current would be observed even in weak fields. Understandably, such a phenomenon is all probability accidental and unstable. However, a similar Landau-Ginzburg equation is obtained for the current in fields $H \sim H_{c1}$, even if no such phase addition takes place, but in this case

$$|\Delta_s| = \lambda_{sd} \sqrt{m_d}\, \Delta_d^{1/2}.$$

If we take into account the deviation of the Fermi surface from a flat surface, for example, if we assume it to be a corrugated plane

$$\varepsilon_d = p_z^2 / 2m_d + \alpha(\cos ap_x + \cos ap_y), \tag{12}$$

(α—coefficient of "corrugation" of the Fermi surface, a—period of the corrugation), then from the usual expansion in terms of the gap we can readily obtain analogously[7]

$$\begin{aligned} eH_{c1}^{\parallel}a^2 &\sim \Delta_d / \alpha, \quad H \parallel z, \\ eH_{c1}^{\perp}a^2 &\sim (\Delta_d / \alpha)^{1/2}, \quad H \perp z. \end{aligned} \tag{13}$$

In these formulas the z axis is perpendicular to the Fermi plane. Since $\Delta_d/\alpha \gg 1$, destruction of superconductivity can occur even in weaker fields $H_0 \sim \Delta_d$, owing to the "moving apart" of the Fermi surface. The analysis agrees with the fact that compounds of the V_3Si group are superconductors of the second kind with high critical fields[8].

In conclusion, the author is sincerely grateful to I. E. Dzyaloshinskiĭ for suggesting the problem and constant guidance of the work.

[1] I. M. Weger, Rev. of Mod. Phys. 36, 1 (1964).
[2] A. P. Levanyuk and R. A. Suris, Usp. Fiz. Nauk 91, 113 (1967) [Sov. Phys.-Usp. 10, 40 (1967)].
[3] J. Labbe and J. Friedel, J. de Phys. 27, 153, 303 (1966).
[4] J. Labbe, J. Friedel, and S. Barisic, Phys. Rev. Lett. 19, 1039 (1967).
[5] Yu. A. Bychkov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. 50, 738 (1966) [Sov. Phys.-JETP 23, 518 (1966)].
[6] J. Labbe, Phys. Rev. 158, 647, 655 (1967).
[7] I. E. Dzyaloshinskiĭ and E. I. Kats, Zh. Eksp. Teor. Fiz. 55, 338 (1968) [Sov. Phys.-JETP 28, 178 (1969)].
[8] C. Shull and F. Wedgwood, Phys. Rev. Lett. 16, 513 (1966).

Translated by J. G. Adashko
69