The superconducting properties and the structural transition in compounds with the *A*-15 lattice

L. P. Gor'kov and O. N. Dorokhov

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
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The dependence of T_c on composition and strain is computed and compared with the corresponding dependence of T_m. It is shown that the superconducting and structural properties of the A-15 compounds can be described, at least qualitatively, in the quasi-one-dimensional model previously developed by the authors. It is assumed that the superconductivity mechanism is analogous to that of the BCS theory. The upper critical field, H_c2, of the V_3Si and Nb_3Sn compounds turns out to be much higher than that of V or Nb.

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1. INTRODUCTION

As is well known (see the reviews[1–3]), the most carefully and thoroughly studied of the entire group of compounds with the β–W structure are, at present, the compounds Nb_3Sn and V_3Si. Among their unusual properties should, first of all, be mentioned the low-temperature, so-called Martensitic, structural transition (of transition points $T_m \approx 49$ and 21–25 K, respectively). This transition is presaged by specific temperature dependences ("precursors"), extending right up to room temperatures, of the magnetic susceptibility and the elastic moduli C_{11} and C_{12}. Both compounds are high-T_c superconductors ($T_c(Nb_3Sn) = 18.2$ K, $T_c(V_3Si) = 17.0$ K). Numerous experimental data (see[1,2]) indicate an interrelationship between their elastic and superconducting properties.

The phenomenological approach[4] uses the assumption that the density of states in the vicinity of the Fermi level has a fine structure—a narrow peak, whose width is estimated from experimental data to be ~ 200 K. The microscopic theories in one form or another are based on the assumption, first noted by Weger,[5] that the chains of transition-element atoms in these compounds play an especial role. In the Labbe–Friedel model[6] and the more simplified RCA model,[7] it is assumed that the bottom of the empty bands of the d electrons localized on these chains is located precisely at the Fermi level for the overlapping s- and p-electron bands. Such an assumption is utterly artificial, and, earlier,[8,9] we developed a detailed microscopic theory of the structural properties of these compounds, considering the above-indicated structural transition to be the result of a special type of the Kohn or Peierls instability in the spectrum of the transverse acoustic phonons.

The purpose of the present paper is to attempt to describe, at least qualitatively, the distinctive features of the superconducting properties of V_3Si and Nb_3Sn. In using the word qualitatively, we have in mind not so much the complexity of the formulas obtained below, as, first and foremost, the well-known irreproducibility of, and the scatter in, the experimental data,[1,10] a circumstance that, strange as it may seem, apparently serves as an argument in favor of our model.

Let us briefly formulate the basic physical assumptions underlying the theory.[8,9] Like Weger,[5] we assume that, in the first approximation, there exists a relatively narrow ($\Delta E \sim 3$–5 eV) one-dimensional band (its origin is connected with the d electrons of the transition-element atoms) for the electrons moving only along the three orthogonal V- or Nb-atom chains. In contrast to[5–7], it is assumed, however, that this band does not overlap other bands (there are no other carriers). The space group symmetry of the A-15 structure guarantees a compulsory degeneracy of the electronic term at the X point.[8] The location of the Fermi level is thereby automatically determined, the number of carriers in the band is large and equal to two (per period of each chain). As has been demonstrated,[8] instability of the structure is already possible in this approximation. The overlap of the electron wave functions among the orthogonal chains of the transition-element atoms is not too small. According to rough estimates (see, for example,[2]), the corresponding overlap integral, B, is of the order of several tenths of an electron volt. Allowance for these effects rectifies the one-dimensional character of the electron spectrum. The characteristic "three-dimensionality" parameter T^* is of second order in B ($T^* \sim B^2/\Delta E$), and is estimated at several hundred degrees K. The three-dimensionality effect can either eliminate altogether the indicated purely one-dimensional Kohn anomaly ("truncate" it at $T \sim T^*$), or leave it, only slightly changing the corresponding transition temperature.[1)] In the latter case (if we abstract ourselves from the possibility of an accidental play on figures) we should expect $T_m \gtrsim T^*$. Since real $T_m \approx 20$–50 K, we choose the first possibility.

A detailed investigation of the structure of the electronic spectrum shows[8] that the electronic density of states is not a constant in the vicinity of the X point of the reciprocal-lattice unit cell and has at energies $\varepsilon_1 = 0$ and $\varepsilon_2 = -2T^*$ two logarithmic peaks of the form

$$\nu(\varepsilon) = \nu(0)\frac{2}{\pi^2}\ln\frac{32T^*}{|\Delta\varepsilon|}, \tag{1}$$

where $\Delta\varepsilon = \varepsilon - \varepsilon_i$ (to the stoichiometric composition corresponds the location of the Fermi level at $\mu = -T^*$).

In our papers,[8,9] the possibility of a structural transition is related with the closeness of the chemical potential (i.e., with the deviation from stoichiometry) to one of the singularities (1). Such an assumption reflects the fact that the appearance of the structural transition depends on the minute details of the preparation of the samples. Of course, deviations from stoichiometry cannot be the only factor responsible for the "fortuity" of the structural transition. The role of impurities requires, of course, an additional investigation.

Below we first formulate the basic equations of the theory of superconductivity in these compounds (more exactly, the equations determining the superconducting-transition temperature) and then investigate the dependence of T_c on composition, the applied strain, and magnetic field, as well as the interrelation between the superconducting and structural transitions. In conclusion, we shall attempt to formulate an answer to the question, repeatedly raised in the literature, whether the high T_c's in these compounds are not the result of a new mechanism of "enhancement of superconductivity by the structural instability" of these systems. Our answer is sooner in the negative.

2. DERIVATION OF THE EQUATIONS FOR THE SUPERCONDUCTING-TRANSITION TEMPERATURE

Below we assume that the nature of the superconductivity in the compounds under consideration is specified by the usual phonon mechanism of the BCS theory: the mutual attraction of the conduction electrons as a result of the exchange of virtual phonons, the Cooper pairs being formed in the singlet state.

Let us recall that the usual method of determining the transition temperature (see, for example,[11]) consists in summing the ladder diagrams of Fig. 1, where a dashed line corresponds to the exchange of a phonon and in the matrix element is represented by the corresponding D function. In the usual single-band BCS model, the matrix element is (leaving out unimportant coefficients) proportional to

$$T\sum_n \int D(p-p')G(p)G(-p)d^3p$$
$$=T\sum_n \int D(p-p')\frac{d^3p}{[i\varepsilon_n-(\varepsilon(p)-\mu)][-i\varepsilon_n-(\varepsilon(p)-\mu)]}$$
$$\to \int D(p-p')\frac{d^3p}{\varepsilon(p)-\mu}\operatorname{th}\frac{\varepsilon(p)-\mu}{2T}=\int D(p-p')\frac{du}{u}\operatorname{th}\frac{u}{2T}\oint\frac{dS}{v_F}.$$

In the last transformation the d^3p integration has been split into integration over the energy variable, $u=\varepsilon(p)-\mu$, within the limits of the Debye cutoff $(-\Theta,\Theta)$, which integration is responsible for the logarithmic intensification of the interaction at low temperatures (the Cooper effect), and integration over the Fermi surface. The

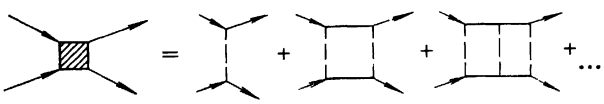

FIG. 1.

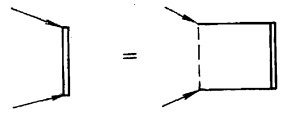

FIG. 2.

latter integration in the anisotropic case is not trivial. The pole of the vertex part determines the superconducting-transition temperature T_c, which is therefore found by solving the homogeneous equation of Fig. 2 for the quantity $\Delta(p)$:

$$\Delta(p)=\int_{-\Theta}^{\Theta} K(pp')\frac{du}{u}\operatorname{th}\frac{u}{2T_c}\oint\frac{dS}{v_F}\Delta(p'). \tag{2}$$

The problem of determining T_c in an anisotropic superconductor was formulated by Pokrovskiĭ[12] in such a form. In (2) $\Delta(p')$ depends only on the position of the momentum p' on the Fermi surface.

Complications in the solution of the analogous problem for the system we are considering occur in two respects: the appearance of a nontrivial dependence on the variable u in the integral over the Fermi surface (the fine structure of the electronic density of states) and the presence of a large number of branches of the energy spectrum. In itself the latter circumstance is not important (two-band models of a superconductor have been studied for diverse reasons by many authors (see, for example,[13]), but it greatly complicates the corresponding equations.

Let us first investigate the shape of the Fermi surface of the electrons. If the interaction between the various chains of atoms is neglected, then the Fermi surfaces are plane and lie near the corresponding faces of the cube of the reciprocal Brillouin zone. Because of the indicated two-fold degeneracy when the position of the Fermi level undergoes small oscillations, the Fermi surface corresponds to either the electron or the hole branch. Allowance for the interaction between the filaments in the main only distorts the shape of the Fermi surface near the corresponding face of the Brillouin zone. The two branches of the spectrum have the form[9] (for the filament along the [001] direction, $\delta_z \equiv \pi/a-p_z$)

$$\varepsilon(p)=T^*\left[\sin^2\frac{p_xa}{2}+\sin^2\frac{p_ya}{2}-2\right]$$
$$\pm\left[(v\delta_z)^2+T^{*2}\left(\sin^2\frac{p_xa}{2}-\sin^2\frac{p_ya}{2}\right)^2\right]^{1/2}. \tag{3}$$

Equation (3) is not applicable near the cube edges, because of the fourfold degeneracy (in the absence of interaction) of the spectral branches, e.g., for the filaments along the z and x axes. For $\varepsilon\sim T^*$, to find the corresponding "curvature" and the Fermi surfaces in this region ($\delta_z=\pi/a-p_z\ll\pi/a$, $\delta_x=\pi/a-p_x\ll\pi/a$), we can use Eq. (10) of[9]:

$$\varepsilon^2[v^2(\delta_x^2+\delta_z^2)+8B^2(1+\cos p_ya)]$$
$$+\varepsilon 4B^2(1+\cos p_ya)va(\delta_x^2+\delta_z^2)-v^4\delta_x^2\delta_z^2=0. \tag{4}$$

It follows from (4) that, in the general case of $\varepsilon \sim T^*$ and $v\delta_z \sim T^*$, the expression (3) becomes inapplicable when $v\delta_x \sim B \propto T^{*1/2}$.

Returning to the problem of the determination of the critical temperature T_c, let us note, first of all, that the diagrammatic equation of Fig. 2 has a complex matrix character, because of the large number (six) of spectral branches figuring in it. In the general form, we have to deal in this equation with Green functions $\hat{G}$ that are 6×6 matrices. We shall denote the elements of the latter by $G^{ik}_{\alpha\beta}$, where the upper pair of indices pertain to the "sort" of filament (i.e., $i, k = x, y, z$), while the lower pair correspond to the choice of the twofold-degenerate representation at the X point. Over the larger part of each of the faces of the Brillouin zone (say, for the x filament), only the diagonal terms, $G^{xx}_{\alpha\beta}$, of the matrix $G^{ik}_{\alpha\beta}$ are, in accordance with (3) and (4), large.

A further simplification of the problem is connected with the assumption that the vertex of a dashed line in Figs. 1 and 2 is diagonal in the index, i, i.e., the scattering of an electron by a virtual phonon does not by itself cause the electron to jump from a filament to a filament. In this case both incoming lines in Fig. 1 have coincident indices (i, i), and we can introduce three "superconducting-gap" matrices: $\Delta^{(x)}_{s\alpha\beta}$, $\Delta^{(y)}_{s\alpha\beta}$, $\Delta^{(z)}_{s\alpha\beta}$.

If we neglect the off-diagonal elements of $G^{ik}_{\alpha\beta}$ with respect to the indices (i, k) in the inner integration of the equation given by Fig. 2, then the problem of the onset of superconductivity turns out to be independent for each of the systems of orthogonal filaments. However, allowance for the off-diagonal elements leads, as we shall see, to the appearance of coupling coefficients that are not too small, as a result of which the superconductivity in these compounds assumes a three-dimensional character.

The phonon-induced attraction is short-range in nature. Nevertheless, the vertices of a dashed line, which correspond to a change in the electron energy when the lattice is deformed in one way or another, generally speaking depend on the phonon wave vector. In the previous papers,[8,9] the Hamiltonian for the electrons of one filament had the form

$$\hat{H} = -a_0\hat{e} + v\delta_z\hat{\tau}_y - c_0\hat{\tau}_x + \hat{V}_{eph},$$
$$a_0 = T^*\left(\cos^2\frac{p_x a}{2} + \cos^2\frac{p_y a}{2}\right), \quad c_0 = T^*\left(\cos^2\frac{p_x a}{2} - \cos^2\frac{p_y a}{2}\right). \tag{5}$$

For the electron-phonon interaction $\hat{V}_{eph}$, we used the expression

$$\hat{V}_{eph} = d_z\varepsilon_{zz}\hat{e} - [d_1(\varepsilon_{xx} - \varepsilon_{yy}) + \gamma u_z]\hat{\tau}_x \tag{6}$$

(the ε_{ik} are the components of the strain tensor and u_z is the sublattice displacement).

The Hamiltonian (6) strictly speaking pertains only to the electron-phonon interaction at $k = 0$. If the phonon wave vector $k \sim \pi/a$, the vertex has the general form

$$V_{eph}(q) = f_1(q)\hat{\tau}_x + f_2(q)\hat{e} + f_3(q)\hat{\tau}_y = \sum_k f_k\hat{\tau}^{(k)} \tag{6'}$$

(f_k is linear in the lattice displacement, and the terms with $\hat{\tau}_z$ would correspond to a representation that is odd in the time: see[8]). The right-hand side of the equation depicted in Fig. 2 for the gap $\Delta^{(i)}_{s\alpha\beta}$ is thus proportional to the following expression:

$$T\sum_\varepsilon \int d^3p' \sum_k \langle f_k^2(q)\rangle \hat{\tau}^{(k)}_{\alpha\gamma}\hat{\tau}^{(k)}_{\beta\delta} \sum_{ll'} \hat{G}^{ll}_{\gamma\mu}(p') G^{ll'}_{\delta\mu'}(-p') \hat{\Delta}^{(l)}_{s\mu\mu'}(p'). \tag{7}$$

Each of the gaps $\Delta^{(i)}_{s\alpha\beta}$ should, since we have assumed Cooper pairing in the singlet state, be symmetric with respect to interchange of the band indices α, β:

$$\hat{\Delta}^{(i)}_s = \alpha^{(i)}_s\hat{e} + \beta^{(i)}_s\hat{\tau}_x + i\gamma^{(i)}_s\hat{\tau}_z. \tag{8}$$

Like Eq. (2), the resulting equations are not soluble in the general form in the case of arbitrary anisotropy of the D functions ($\langle f^2(q)\rangle$). We shall restrict ourselves to the approximation in which, as a result of the electron-phonon exchange, only the electrons located on one and the same chain interact. In this case $\Delta^{(i)}_s(p)$ does not depend on the position of the vector p on the Fermi surface.

Let us consider the filament along the x axis and investigate first the diagonal (in i, l) terms in the expression (7). As has been shown,[9] the Green functions $\hat{G}^{ii}(p)$ have (in the notation used in[9]) the form

$$\hat{G}^{ii}(p) = [(i\varepsilon_n + a)\hat{e} + v\delta_i\hat{\tau}_y - c_i\hat{\tau}_x][(i\varepsilon_n + a)^2 - (v\delta_i)^2 - c_i^2]^{-1}, \tag{9}$$
$$\delta_i = \pi/a - p_i,\ a = T^*(\cos^2\varphi + \cos^2\psi) - \mu,\ c_i = T^*(\cos^2\varphi - \cos^2\psi) - \Delta_i$$

(the tetragonal distortion $a/c - 1 = \alpha$, $\varepsilon_{xx} = \varepsilon_{yy} = \alpha/3$, $\varepsilon_{zz} = -2\alpha/3$, $\Delta_x = -\Delta_y = d_1\alpha$, $\Delta_z = 0$). After the substitution of (9) into (7) and simple matrix transformations, the diagonal—in (i, l)—part of (7) assumes the following form:

$$T\sum_n \int d^3p\{A(\varepsilon_n, p)\hat{e} + B(\varepsilon_n, p)\hat{\tau}_x + C(\varepsilon_n, p)i\hat{\tau}_z\}$$
$$\times[(i\varepsilon_n + a)^2 - (v\delta_i)^2 - c_i^2]^{-1}[(-i\varepsilon_n + a)^2 - (v\delta_i)^2 - c_i^2]^{-1},$$

where, as in the BCS theory (see the derivation of (2) above), the denominators of the Green functions give rise to terms logarithmically dependent on temperature, while the expressions A, B, and C have the following form:

$$A(\varepsilon_n, p) = \{[a^2 + \varepsilon_n^2 + (v\delta_i)^2 + c_i^2]\alpha^{(i)}_s - 2ac_i\beta^{(i)}_s\}[\langle f_1^2\rangle + \langle f_2^2\rangle + \langle f_3^2\rangle],$$
$$B(\varepsilon_n, p) = \{-2ac_i\alpha^{(i)}_s + [a^2 + \varepsilon_n^2 - (v\delta_i)^2 + c_i^2]\beta^{(i)}_s\}[\langle f_1^2\rangle + \langle f_2^2\rangle - \langle f_3^2\rangle],$$
$$C(\varepsilon_n, p) = \{a^2 + \varepsilon_n^2 - (v\delta_i)^2 - c_i^2\}\gamma^{(i)}_s[-\langle f_1^2\rangle + \langle f_2^2\rangle + \langle f_3^2\rangle]. \tag{10}$$

We see, first of all, that the terms with $\gamma^{(i)}_s$ in (8) split off from $\alpha^{(i)}_s$, $\beta^{(i)}_s$.

The next complicated problem consists in the fact that in the expressions (10) the factors $\langle f_i^2\rangle$ enter in combinations with different signs. Let us recall in this connection that the quantities f_i in (6') are linear in the lattice displacements, i.e., the mean values $\langle f_i^2(q)\rangle$ are proportional to the corresponding D functions, and, therefore, as is usual in the phonon mechanism, the + sign in front of $\langle f_i^2\rangle$ corresponds to attraction in the Cooper effect. In $\langle f_i^2(q)\rangle$, at small phonon wave vectors q, the

quantity $\langle f_1^2\rangle \propto d_1^2$, $\langle f_2^2\rangle \propto d_2^2$, and $\langle f_3^2\rangle$ is, in general, absent. An analysis of the behavior of the elastic moduli[9] convinced us that, in any case, d_2 is substantially less than d_1. The experimental facts,[1] which indicate an interrelation between the structural and superconducting transitions, clearly reflect the special role played in the phenomenon of superconductivity in these compounds by the acoustic phonon branches determining the moduli C_{11} and C_{12}. On these grounds, we consider it possible to retain in (10) only the terms with $\langle f_1^2\rangle$ and in (8) only the first two terms. Since, according to the neutron experiments,[14,15] the maximum frequencies of the acoustic phonons in the compounds V_3Si and Nb_3Sn do not exceed 200 K, we shall also assume that the corresponding Debye cutoff Θ in the integrals over the energy variable (see Eq. (7)) is small in comparison with T^*. Of course, such a procedure implicitly contains the assumption that the electron-phonon interaction is weak, whereas the high T_c's in these compounds point rather to the opposite situation. We shall see, however, that even under these simplifications from the model follow several important assertions that are at least qualitatively valid.

For an arbitrary position of the chemical potential $\mu \sim T^*$ (deviation from stoichiometry), the Fermi surface is determined by the equation $\mu = \varepsilon_i(p)$, where ε_i is one of the electronic branches (3). Its deviation from the plane of the Brillouin face (for the filament along the x axis) is $\delta_x \sim T^*/v$.

After the corresponding simplifications in (10) with the use of the condition $\varepsilon_i(p) \approx \mu$, the right-hand side of the equation depicted by Fig. 2, or, more exactly, the diagonal—in (i, l)—terms of the expression (7) assume the form

$$R\frac{4}{\pi^2}\int_{-\Theta}^{\Theta}\frac{du}{2u}\operatorname{th}\frac{u}{2T} \times \int_0^{\pi/2}\int_0^{\pi/2} d\varphi\, d\psi \frac{a[(\alpha_s^{(i)} - c_i\beta_s^{(i)}/a)\hat{e} + (c_i^2\beta_s^{(i)}/a^2 - c_i\alpha_s^{(i)}/a)\hat{\tau}_x]}{(u+\mu+\Delta_i+2T^*\cos^2\varphi)^{1/2}(u+\mu-\Delta_i+2T^*\cos^2\psi)^{1/2}}. \quad (11)$$

The requirement that the radicands be positive determines the integration domains for (φ, ψ). The coefficient R contains both the diagram coefficients and the interaction $\langle f_1^2\rangle$; the factor $4/\pi^2$ has been chosen for the normalization of the integral over the Fermi surface to the area of the face of the reciprocal Brillouin zone.

In the general case of $\mu \sim T^*$, the strains $\Delta_i = d_1\alpha$ enter into Eq. (11), determining the transition temperature T_c, only side by side with the scale T^*. The situation changes if the chemical potential is chosen to be close to one of the singularities, (1), in the electronic density of states.[2)] In accordance with our results,[9] the quantity $T_m^0 \sim T_c \ll T^*$, Θ becomes the characteristic scale for the variation of μ and Δ.

In evaluating the integrals in (11), it is convenient to introduce under the logarithm $X = \ln(2\gamma\Theta/\pi T)$ the same combination of numerical factors that, for the chosen method of truncation, figures in the BCS theory, and rewrite (11) in terms of the matrix $\hat{K}^{(i)}$. The equation depicted by Fig. 2 has the form

$$\begin{Bmatrix}\alpha_s^{(i)}\\ \beta_s^{(i)}\end{Bmatrix} = \frac{R}{\pi^2}\hat{K}^{(i)}\begin{Bmatrix}\alpha_s^{(i)}\\ \beta_s^{(i)}\end{Bmatrix}, \quad (12)$$

where for $K^{(i)}$, after the computations, we obtain

$$\hat{K}^{(i)} = \begin{Bmatrix} P(X) - \frac{1}{2}\left[F\left(\frac{\mu-\Delta_i}{2T}\right) + F\left(\frac{\mu+\Delta_i}{2T}\right)\right], & \frac{1}{2}\left[F\left(\frac{\mu-\Delta_i}{2T}\right) - F\left(\frac{\mu+\Delta_i}{2T}\right)\right] \\ \frac{1}{2}\left[F\left(\frac{\mu-\Delta_i}{2T}\right) - F\left(\frac{\mu+\Delta_i}{2T}\right)\right], & P(X) - \frac{1}{2}\left[F\left(\frac{\mu-\Delta_i}{2T}\right) + F\left(\frac{\mu+\Delta_i}{2T}\right)\right] - 8GX \end{Bmatrix}, \quad (13)$$

Here we have used the following notation:

$$P(X) = X^2 + 2X\ln\frac{32T^*}{\Theta} + C_1, \qquad C_1 = -\ln^2\frac{\pi}{4\gamma} + \int_0^\infty \ln^2 u \operatorname{ch}^{-2} u\, du \approx 1.32, \quad (13')$$

$$F(z) = \int_0^\infty \frac{du}{u}\operatorname{th}(|z|u)\ln\left|1 - \frac{1}{u^2}\right|$$

($G = 0.916$ is the so-called Catalan constant). The appearance of the factor π^{-2} justifies to a certain extent our truncation procedure—the same as in the BCS theory. It is appropriate here to note at once that if we chose a chemical potential $\mu \gg T^*$, then we should, in accordance with (11) and (2), have obtained in place of (12) and (13)

$$\alpha_s^{(i)} = R'X\alpha_s^{(i)}. \quad (14)$$

The coupling constant R', as has already been pointed out,[9] differs, of course, from R in (12). Below we shall return to the discussion of this question.

The Eqs. (12) would determine the superconducting-transition temperature for each filament separately if there were no coupling between them. The computation of the corresponding coupling coefficients is carried out in the Appendix. Forming the column $\{\Psi\}$ from the three columns

$$\begin{Bmatrix}\alpha_s^{(i)}\\ \beta_s^{(i)}\end{Bmatrix}$$

for each of the filaments, we obtain the complete matrix equation from which we should determine the temperature of transition into the superconducting state:

$$\{\Psi\} = R\pi^{-2}\hat{K}\{\Psi\}. \quad (15)$$

In order not to write out the entire matrix, let us give only the component of Eq. (15) for the filament along the x axis:

$$\begin{Bmatrix}\alpha_s^{(x)}\\ \beta_s^{(x)}\end{Bmatrix} = \frac{R}{\pi^2}\hat{K}^{(x)}\begin{Bmatrix}\alpha_s^{(x)}\\ \beta_s^{(x)}\end{Bmatrix} + \frac{RX}{\pi^2}\begin{Bmatrix}k_1 & k_1\\ k_2 & k_2\end{Bmatrix}\begin{Bmatrix}\alpha_s^{(y)}\\ \beta_s^{(y)}\end{Bmatrix} + \frac{RX}{\pi^2}\begin{Bmatrix}k_1 & -k_1\\ -k_2 & k_2\end{Bmatrix}\begin{Bmatrix}\alpha_s^{(z)}\\ \beta_s^{(z)}\end{Bmatrix}, \quad (16)$$

where the coefficients $k_1, k_2 \propto (T^*/\Delta E)^{1/2}$ are given by the formulas (A.3, 3′) of the Appendix. The remaining components of Eq. (15) are obtainable from (16) by cyclic permutation.

3. DEPENDENCE OF T_c ON COMPOSITION AND STRAIN. THE CRITICAL FIELD

Let us proceed to analyze the obtained equations. First of all, let us note that the coupling between the individual filaments is by no means weak. Indeed, the relative order of magnitude of the terms with k_1 and k_2 in Eq. (16) in comparison with the dominant terms is

$$(k_1, k_2) \Big/ \left(\ln\frac{2\gamma\Theta}{\pi T_c} + 2\ln\frac{32T^*}{\Theta}\right) \sim \left(\frac{T^*}{\Delta E}\right)^{1/2}. \tag{17}$$

Below we shall attempt to estimate the quantity T^* more exactly, but it is already clear from the foregoing that (17) has a value of about 0.1.

Let us note the close relationship between the obtained expressions in (13) and the dependence, found earlier in[9], of the elastic moduli on temperature and strain. Let us differentiate, for example, the diagonal element $K_{11}^{(i)}$ of the matrix (13) with respect to temperature:

$$\frac{\partial K_{11}^{(i)}}{\partial T} = -\frac{2}{T}\left\{\ln\frac{T_m^0}{T} + \frac{1}{2}\left[s\left(\frac{\mu-\Delta_i}{T}\right) + s\left(\frac{\mu+\Delta_i}{T}\right)\right] + \ln\frac{64\gamma T^*}{\pi T_m^0}\right\}. \tag{18}$$

(Here $s(x)$ is a function introduced in[9].)

For the filaments affected by the tetragonal transition (if $T_c < T_m$) or by external strain, the first three terms are exactly proportional to the elastic modulus C_s (see Eq. (24) in[9]) in the deformed phase, which modulus is, generally speaking, small at low temperatures. The last term therefore has the meaning of the unrenormalized modulus C_s, i.e., it is proportional to $C_s(T \sim T^*)$.

We shall also need below the asymptotic expressions for the function $F(z)$, (13′):

$$F(z) \approx \begin{cases} 7\zeta(3)z^2/\pi^2, & z \ll 1, \\ \ln^2(4\gamma z/\pi) - \pi^2/6 + C_1, & z \gg 1. \end{cases} \tag{19}$$

The general equation (16) has, strictly speaking, six solutions for the critical temperature of transition into the superconducting state. Evidently, only the largest of these values plays a role. In the first approximation the magnitude of the transition temperature already can be estimated from Eq. (12). The role of the terms with (k_1, k_2) in (16) consists in providing corrections $\propto (T^*/\Delta E)^{1/2}$ to the thus obtained transition temperature. These terms are by no means small, which has already been indicated above; furthermore, they remove the degeneracy that we should have in the case of three independent filaments, and guarantee the requisite symmetry of the superconducting gap in the cubic or tetragonal phase.

To obtain physical results, we can further simplify Eq. (16). In fact, analyzing the structure of the matrix (13), we see that the term $K_{11}^{(i)}$ is greater than $K_{22}^{(i)}$ by the quantity $8GX$. Therefore, the compensation for the smallness of R/π^2 by the quantity $K^{(i)}$ in (12) occurs, first and foremost, for $K_{11}^{(i)}$, and it follows from this that the order of magnitude of $\beta_s^{(i)}$ in comparison with $\alpha_s^{(i)}$ is either

$$\beta_s^{(i)} \sim \left\{F\left(\frac{\mu-\Delta_i}{2T}\right) - F\left(\frac{\mu+\Delta_i}{2T}\right)\right\}\frac{\alpha_s^{(i)}}{16GX}$$

or

$$\beta_s^{(i)} \sim k_2\alpha_s^{(i)}/8G,$$

i.e., $\beta_s^{(i)}$ is always at least an order of magnitude smaller than $\alpha_s^{(i)}$.

Let us first consider T_c in the cubic phase. Let in the absence of external influences (strains; magnetic fields) the transition temperature $T_c(\mu)$ be known. Equation (15)

$$\{\Psi_c\} = R\pi^{-2}\{\hat{K}_{cub}\}\{\Psi_c\} \tag{15′}$$

determines the corresponding column $\{\Psi_c\}$ at $T = T_c(\mu)$. If the matrix $\hat{K}$ is subjected to some perturbation on account of, for example, deformations:

$$\hat{K} = \hat{K}_{cub} + \hat{K}_1,$$

the small change in the temperature is determined by the usual orthogonality condition

$$\{\Psi_{cub}\}\cdot\left[\Delta T_c\frac{\partial\hat{K}_{cub}}{\partial T} + K_1\right]\{\Psi_{cub}\} = 0. \tag{20}$$

Using (18) and the relation

$$\frac{\partial F(x)}{\partial x} = -\frac{2}{x}s(2x),$$

as well as the equality of all the $\alpha^{(i)}$ in the cubic phase, we obtain from (20) and (18) ($\mu \lesssim T_m^0$)

$$\frac{\Delta T_c}{T_c(\mu)} = -\frac{1}{3}\ln^{-1}\left(\frac{64\gamma T^*}{\pi T_c}\right)\frac{\Delta^2}{\mu^2}\left\{s\left(\frac{\mu}{T}\right) - \frac{\mu}{T}s'\left(\frac{\mu}{T}\right)\right\} < 0, \tag{21}$$

where in (18) we have retained only the large logarithmic term. For $\mu = 0 (T_c \equiv T_c^0)$

$$\frac{\Delta T_c}{T_c^0} = -\frac{7\zeta(3)}{12\pi^2}\left(\frac{\Delta}{T_c^0}\right)^2\ln^{-1}\left(\frac{64\gamma T^*}{\pi T_c^0}\right). \tag{21′}$$

The expression for the change in the Martensitic-transition temperature follows from Eq. (24) (see[9])

$$\frac{\Delta T_m}{T_m^0} = -\frac{7\zeta(3)}{4\pi^2}\left(\frac{\Delta}{T_m^0}\right)^2. \tag{22}$$

Although there are no quantitative data for $dT_m/d\alpha$, it is well known that T_c is much less sensitive to strains than T_m.

In the tetragonal phase, or, accordingly, in a deformed sample the symmetry of the superconducting phase leads to the appearance of an anisotropy in the gap. Within the accuracy in which it is possible to neglect $\beta_s^{(i)} \ll \alpha_s^{(i)}$, Eq. (16) constitutes a third-order algebraic system. The simple determinant can easily be computed in the general form: From the three roots of the equation

$$\det\begin{Vmatrix} K_{11}^{(x)} - \pi^2/R & k_1X & k_1X \\ k_1X & K_{11}^{(y)} - \pi^2/R & k_1X \\ k_1X & k_1X & K_{11}^{(z)} - \pi^2/R \end{Vmatrix} = 0 \tag{23}$$

should be chosen that which gives the highest T_c. We assume that the deformation affects the (x, y) filaments and, therefore, $K_{11}^{(x)} = K_{11}^{(y)}$ and differ from $K_{11}^{(z)}$ by the dependence of the terms with F, (13′), on Δ.

In accordance with our general idea that the structural transition is possible when the position of the chemical potential coincides with a singularity in the electronic density of states, (1), the effects of the tetragonal anisotropy of the superconducting gap should be sought in samples that undergo the transition, or that exhibit appreciable softening of the elastic modulus C_s, i.e., when $\mu \sim T_m^0$. In this case, since $\Delta = d_1\alpha$ is also of the order of T_m^0, the anisotropy of the superconducting gap Δ_s can become of the order of unity. The most interesting situation arises in that limiting case when the superconductivity is studied in a good (in the indicated sense) sample that is highly deformed by applied external strains α: the quantity $\Delta = d_1\alpha \gg T_m^0$. The superconductivity in this case appears, first and foremost, in the z filament, the electronic spectrum of which is not affected by the deformation (the transition temperature T_c, however, drops slightly (see below)). The magnitude of the anisotropy is determined by the ratio

$$\alpha_s^{(x)} = \alpha_s^{(y)} = \lambda\alpha_s^{(z)} = k_1 X \alpha_s^{(z)} / F(\Delta/2T). \tag{24}$$

Using the asymptotic form of $F(z)$, (19), for $z \gg 1$, let us write down for the coefficient $\lambda(\Delta)$ in (24) the explicit expression

$$\lambda(\Delta) = k_1 \ln\left(\frac{2\gamma\Theta}{\pi T_c}\right) \Big/ \ln^2\left(\frac{2\gamma\Delta}{\pi T_c}\right). \tag{24′}$$

This condition requires strains that are an order of magnitude greater than the spontaneous strains that arise in the structural transformations occurring in V_3Si ($\alpha \approx -2.2\times10^{-3}$) and Nb_3Sn ($\alpha \approx 6\times10^{-3}$), since, in general, when the large coefficients in k_1, (A.3), are taken into account, the quantity k_1 has a value of several tenths.

Above we mentioned that the corresponding T_c drops. Indeed, looking over the roots of Eq. (23), we see that, in the absence of deformation, the transition temperature is determined by the equation

$$\pi^2/R = P(X) - F(\mu/2T) - k_1 X, \tag{25}$$

whereas in the limit (24′) the third term on the right-hand side of (25) is absent. Combining with (18), we obtain the estimate

$$\frac{\Delta T_c}{T_c} \approx \frac{k_1}{2} \ln\left(\frac{2\gamma\Theta}{\pi T_c}\right) \Big/ \ln\left(\frac{64\gamma T^*}{\pi T_c}\right),$$

which shows that in a polycrystal or in a sample in which the internal strains have not been eliminated, T_c can be appreciably lower for the given composition.

Equation (25) allows us to investigate the behavior of T_c as a function of composition (μ). For small deviations of μ, we obtain ($T_c^0 \equiv T_{c\mu}$ for $\mu = 0$)

$$\frac{\Delta T_{c\mu}}{T_c^0} = -\frac{7\zeta(3)}{8\pi^2}\left(\frac{\mu}{T_c^0}\right)^2 \Big/ \ln\left(\frac{64\gamma T^*}{\pi T_c^0}\right). \tag{26}$$

In the limit of large μ, using the asymptotic expression of $F(z)$, we find

$$\ln\frac{T_c^0}{T_{c\mu}} = \left[\ln^2\left(\frac{2\gamma\mu}{\pi T_c^0}\right) - \frac{\pi^2}{6} + C_1\right] \Big/ 2\ln\left(\frac{64\gamma T^*}{\pi T_c^0}\right). \tag{27}$$

It follows from (26) and (27) that, in contrast to the structural transition, the existence of which is limited to the region $\mu \sim T_m^0$, the superconductivity also occurs under conditions when μ is significantly removed from the position near the peak in the density of states. Furthermore, because of the substantial logarithms in the denominators of both expressions, the change in T_c is relatively small. These results are, of course, in accord with what is observed experimentally.

In conclusion of this section, let us derive an equation determining the upper critical field H_{c2} in the vicinity of the transition point.[3)] For its derivation, it is necessary to write (7) for the variable in the coordinates: $\Delta_s(R)$. In terms of the Fourier components, this approximation implies the substitution in (7)

$$\hat{G}(p)\hat{G}(-p) \to \hat{G}(p)\hat{G}(q-p)$$

and the subsequent expansion in q up to terms of the form $(qv/T_c)^2$ inclusively,[17] where

$$\hat{\mathbf{q}} = (-i\nabla - 2e\mathbf{A}(x)/c).$$

A simple calculation for the component $K_{11}^{(z)}$ adds to the matrix (12), (13) the following term:

$$-7G\zeta(3)v^2q_z^2/4\pi^2T^2. \tag{28}$$

This coefficient has been derived up to the terms of $(\mu/T^*, \Delta/T^*)$, i.e., (28) depends weakly on the details of the fine structure of $\nu(\varepsilon)$. (The remaining effective masses are very large because of the smallness of $T^*/\Delta E$.)

We obtain the equation for the Ginzburg–Landau wave function $\Psi(x) = \psi(x)\{\lambda, \lambda, 1\}$ immediately in the tetragonal phase ($\lambda < 1$) from an orthogonality relation of the type (20):

$$\Delta T\left(\frac{\partial K_{11}^{(z)}}{\partial T} + 2\lambda^2\frac{\partial K_{11}^{(x)}}{\partial T}\right)\psi - \frac{7G\zeta(3)v^2}{4\pi^2T^2}\left\{\left(-i\frac{\partial}{\partial z} - \frac{2eA_z}{c}\right)^2 + \lambda^2\left(-i\tilde{\nabla} - \frac{2e\tilde{A}}{c}\right)^2\right\}\psi = 0, \tag{29}$$

where the sign ~ denotes a vector in the (x, y) plane. The quantity λ determines the anisotropy of the field: $H_{c2\perp} \propto \lambda^{-1}$, $H_{c2\parallel} \propto \lambda^{-2}$. In the BCS theory we have[17]

$$\frac{48\pi^2T_c^2}{7\zeta(3)v_F^2}\left(\frac{T_c - T}{T_c}\right)\psi(r) + (\hat{p} - 2e\hat{A})^2\psi(r) = 0.$$

If we reduce (29) to the same form, then the term $\propto (T_c - T)/T_c$ has the form (in the cubic phase)

$$\frac{48\pi^2T_c^2}{7\zeta(3)v_F^2} \to \frac{48\pi^2T_c^2}{7\zeta(3)v^2}\frac{1}{2G}\left\{\ln\frac{T_c^0}{T_c} + s\left(\frac{\mu}{T_c}\right) + \ln\frac{64\gamma T^*}{\pi T_c^0}\right\}. \tag{30}$$

Purely qualitatively comparing, for example, Nb with Nb_3Sn, we see that, owing to the high T_c's and densities of states (lower v's and a substantial logarithmic factor), the critical fields in the A-15 compounds increase by at least an order of magnitude irrespective of the effect of the ordinary impurity mechanism.

Finally, let us attempt to estimate T^*, comparing Testardi's data (see[11]) for the dependence of T_c on strain in the compound V_3Si, $T_c(\alpha) - T_c^0 \approx -\frac{20}{3}\times 10^4 \alpha^2 K$, with the formula (21), where $\Delta = d_1\alpha$. Taking $d_1 \approx 1$ eV,[4)] we obtain $\ln(64\gamma T^*/\pi T_c^0) \approx 7-7.4$ and T^* between 550 and 800 K, the estimate being, of course, rather arbitrary, in view of the fact that we used formulas with $\mu = 0$.

4. CONNECTION OF T_c WITH THE STRUCTURAL TRANSITION

The results of the investigations of $A_3B_{1-x}C_x$-type alloys of the A-15 group of compounds (see[11]), as well as the results of the study of the properties of these compounds as a function of the deviation in them from the stoichiometric composition (for V_3Si see[19]), amount qualitatively to the following. Small changes in composition ($x \sim 0.1$) are capable of freezing the structural transition in the system. Usually, the maximum T_c then occurs at the limit (with respect to composition) of the cubic phase. The changes in T_c are then small and vary from 0.1 to 1 K. In the paper by Berthel *et al.*,[19] it is reported that at one of the existence boundaries for the tetragonal phase of V_3Si the quantity T_c decreases sharply, with $\Delta T_c \approx 0.3$ K. In the literature these facts are regarded as confirmation of the existence of some new hypothetical mechanism of "superconductivity enhancement on account of lattice instability," the point at which the maximum T_c is realized in the cubic phase being interpreted as the moment of maximum instability, frozen in by the presence of the impurity.

We shall show in this section that all these effects are easily explained in the framework of the phonon mechanism of the usual BCS theory in accordance with the above-obtained formulas, and are only a consequence of the nearness of the two transition points. Moreover, the results obtained by Berthel *et al.*[19] should evidently rather be regarded as the first experimental confirmation of the fact that the structural transition in V_3Si is, as it should be,[20] a first-order transition.

In order to explain this idea, we schematically show two curves in Fig. 3. The first shows $T_m(\mu)$, the structural-transition temperature as a function of composition, its broken part having been computed as if no superconductivity occurred in the system. Similarly, the dashed part of the second, flatter curve for T_c corresponds to Eq. (25) without allowance for tetragonal distortions. At the point, μ^*, of their intersection, if the structural phase transition is of first order, a spontaneous finite strain arises discontinuously and the change in T_c is given by the expression (21).

It remains to show that in our theory the phase transition is indeed of first order. Before proceeding to this, we should have constructed the two curves and found μ^*. However, $T_c(\mu)$ contains two parameters, T^* and Θ,

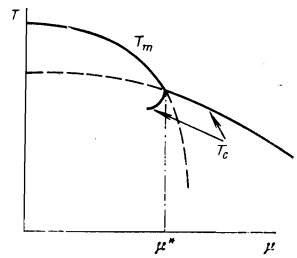

FIG. 3.

that, unfortunately, cannot be determined to any degree of accuracy in the existing experimental situation. Therefore, we are obliged to consider two cases: $\mu^*/T_m^0 \ll 1$ and $\mu^*/T_m^0 \sim 1$. It is interesting to note that the mechanisms making the structural transition a first-order transition in the two cases are different.

Let us begin with the case $\mu/T_m^0 \ll 1$. The formulas (14), (16), and (26) from[19] described, for small μ, the structural transition as a second-order transition. Meanwhile, it is not difficult to see that the group of symmetry transformations for the A-15 lattice admits of the third-order invariant

$$\varepsilon_{xx}(\varepsilon_{yy}-\varepsilon_{zz})^2+\varepsilon_{yy}(\varepsilon_{zz}-\varepsilon_{xx})^2+\varepsilon_{zz}(\varepsilon_{xx}-\varepsilon_{yy})^2.$$

Such invariants of the Landau expansion for the thermodynamic potential indeed arise, but they are connected with the d_2 terms in the electron-strain interaction, terms that, according to our estimates,[9] are appreciably smaller than d_1. Taking them into account, and setting $\vartheta = d_2/d_1 \ll 1$, we obtain the following expansion for the thermodynamic potential near the transition point in the tetragonal phase:

$$\delta\Omega = -\frac{2\nu(0)}{3\pi^2}\left\{\left[\ln\frac{T_m^0}{T}+s\left(\frac{\mu}{T}\right)\right]\Delta^2 - \frac{\vartheta}{3}s'\left(\frac{\mu}{T}\right)\frac{\Delta^3}{T}+\frac{1}{12}s''\left(\frac{\mu}{T}\right)\frac{\Delta^4}{T^2}\right\}. \quad (31)$$

For small ϑ, the shift in the temperature as a result of a change in the nature of the phase transition is proportional to ϑ^2; therefore, T_m is determined as before by the equation

$$\ln(T_m^0/T_m)+s(\mu/T_m)=0,$$

while the spontaneous strain, α_{sp}, is, as can easily be verified, equal to

$$d_1\alpha_{sp} = \frac{2T_m\vartheta s'(\mu/T_m)}{s''(\mu/T_m)}. \quad (32)$$

For small μ/T_m

$$\alpha_{sp} = 2\vartheta\mu/d_1. \quad (32')$$

We have, however, already noted[9] that the phase transition turns out to be a first-order transition irrespective of the above-expounded mechanism if μ is sufficiently large. In particular, this is evident already from (31), since the function $s''(\mu/T)$ passes through

zero at $\mu/T = x_0 = 1.91$ and becomes positive. In this case we can drop in (31) the term with $\vartheta \ll 1$, but then the expansion (31) is itself already inapplicable.

The calculation of the thermodynamic potential with the aid of the formula (16) from[9] would require numerical computations. Since there are a number of neglected factors in our theory (see below), we restricted ourselves to only the $T = 0$ case. In this limit the thermodynamic potential can be computed explicitly:

$$\delta\Omega = \frac{\nu(0)}{3\pi^2}\left\{(\mu+\Delta)^2 \ln\frac{2\gamma|\mu+\Delta|}{\pi e^{1/2} T_m^0} + (\mu-\Delta)^2 \ln\frac{2\gamma|\mu-\Delta|}{\pi e^{1/2} T_m^0} - 2\mu^2 \ln\frac{2\gamma|\mu|}{\pi e^{1/2} T_m^0}\right\}. \quad (33)$$

The quantity Δ itself as a function of μ is determined from the equilibrium condition $\partial\delta\Omega/\partial\Delta = 0$. The form of the solution, shown in Fig. 4, indeed shows that, as $|\mu|$ decreases, the cubic state discontinuously goes over into the tetragonal phase. The value $\mu_{cr} = 1.32\,\mu_c'$ ($\mu_c' = \pi T_m^0/2\gamma$) is determined numerically by the condition $\delta\Omega(\mu, \Delta(\mu)) = 0$; the quantity $\Delta(\mu_{cr}) = 2.27\,\mu_c'$, $\Delta(0) = e\,\mu_c'$. In order to find the observed[19] value of ΔT_c from (21), all the computations should be carried out at finite temperatures.

According to (32) and (32′), the sign of the tetragonal strain depends on the combination μd_2, i.e., it can vary with composition; we obtain the same result if the terms with d_2 are included in (33) as small corrections. This variation has indeed been observed in $Nb_3Sn_{1-x}Sb_x$.[21]

When we spoke about a number of neglected factors, we, in particular, had in mind the fact that both above and in the earlier paper[9] the interactions with the displacements of the sublattices of the transition-element atoms were, for simplicity, neglected. These displacements and the strain terms with d_1 transform according to the same representation.[8] We have not studied how the neglected terms affect the obtained result.

The accuracy with which the composition of the alloy $Nb_3Sn_{1-x}B_x$ (B = Sb,[21] Al[22]) is controlled clearly does not exceed 1%. If we assume that, as compared with the Sn atom with respect to the number of electrons in the unfilled shell, Sb or Al simply adds or removes one conduction electron, then the change, $\delta\mu$, in the Fermi level is given by

$$8\delta\mu\nu(0) \approx 2x,$$

where for Nb_3Sn an estimate[9] gives $\nu(0) \approx 6.7$ (eV-at)$^{-1}$. In this case $x \sim 1\%$ corresponds to

$$\delta\mu \sim \frac{10^{-2}}{4\cdot 6.7}\,\text{eV} \approx 4\text{K}.$$

In Vieland's paper,[21] $x \approx 0.15$, i.e., $\delta\mu \sim 60$ K; in Vieland and Wicklund's work,[22] the existence boundary for the tetragonal transition corresponds to $x \approx 0.075$, i.e., $\delta\mu \sim 30$ K.

In conclusion, let us consider the question: Under which conditions can we expect the highest T_c in a given superconductor. If the material is capable of undergoing a low-temperature structural transition, then ignoring the lowering of T_c as a result of the spontaneous deformation arising in the Martensitic transition (see Fig. 3), the formula of the preceding section for T_c, and the ideas of our earlier paper,[9] according to which the coupling constant R (which is proportional to λ_{eff}[9]) is maximal because of the phonon softening in the same region, we have that the highest T_c's correspond to proximity to one of the peaks in the density of states (2). The internal strains in the crystal play a negative role.

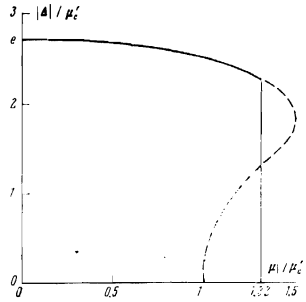

FIG. 4.

The dimensionless coupling constants in these materials are by no means small,[5)] $\Theta \sim T^*$, and into the softening of the elastic moduli and into the interaction responsible for the electron Cooper pairing enter close quantities. From this point of view, the closeness of T_c and T_m is not surprising, although the situation is possible in which $T_m < T_c$, as, for example, in Nb_3Al.[1] The closeness of T_c and T_m could be a consequence of the specific properties of the one-dimensional model, as has earlier been pointed out.[8] The case in which the controlling transition parameter is connected with the electrons requires a special investigation.

The foregoing comments pertain to the variation of the chemical composition (μ) near stoichiometry within limits $\sim T^*$. If, as in Eq. (14), $\mu \gg T^*$, then the constant R' already differs significantly from R as a result of the "parquet" effects connected with the one-dimensionality of the filaments.[8] This behavior does not lend itself to a simple quantitative analysis.

Finally, let us once more repeat that in the investigated model the variation of composition amounts to the "pouring" of electrons into the hard energy zone. This is the principal approximation of the theory, and the role of impurities requires a special investigation.

APPENDIX

To compute the coefficients coupling the superconducting gaps in the various filaments, we need the off-diagonal—in the filament indices—elements of the Green function. These elements are large only in the vicinities of the edges or vertices of the reciprocal-unit-cell cube, where the electron spectrum in the absence of interaction is respectively fourfold or sixfold degenerate. The corners of the cube make a small contribution. Therefore, let us consider, for example, the cube edge at which the electronic terms of the filaments along the x and y axes join. The $\det \| \hat{G}_0^{-1} \|$ (see Eq. (4)) was

computed earlier[9] in a small neighborhood of this edge. For the determination of the off-diagonal minors of the matrix $\hat{G}$, it is sufficient to use the form of $\hat{G}_0^{-1}$:

$$\hat{G}_0^{-1} = \begin{Vmatrix} i\varepsilon_n+\mu & i\delta_x v & B_z & -B_z \\ -i\delta_x v & i\varepsilon_n+\mu & B_z & -B_z \\ B_z^* & B_z^* & i\varepsilon_n+\mu & iv\delta_y \\ -B_z^* & -B_z^* & -iv\delta_y & i\varepsilon_n+\mu \end{Vmatrix}. \quad (A.1)$$

(Only the quantities $|B_z|^2 = 2B^2(1+\cos p_z a)$ enter into the answer below.) In the indicated region all the terms in the matrix $\hat{G}_0^{-1}$ that have a structure $\sim B^2 \propto T^*$ contain additional small factors, owing to the small δ_x and δ_y. Furthermore, in accordance with (4), the dominant contribution to the integrals (7) from the off-diagonal terms is connected with the regions $B/v \sim |\delta_x| \gg |\delta_y|$ or $|\delta_y| \sim B/v \gg |\delta_x|$.

The determinant of the fourth-order matrix $\hat{G}_0^{-1}$ for $\mu \sim T^*$ has the form

$$\det \|G_0^{-1}\| = [i\varepsilon_n - (\varepsilon_1 - \mu)][i\varepsilon_n - (\varepsilon_2 - \mu)][(v\delta_x)^2 + (v\delta_y)^2 + 4|B_z|^2],$$

where ε_1 and ε_2 are the roots of Eq. (4). Let us proceed to the computation of the minors of the matrix inverse to (A.1) for $\delta_y \gg \delta_x$, for example. Since the integration in (7) is performed along the Fermi surface (let its equation be $\varepsilon_1 - \mu = 0$), we obtain the Green function $\hat{G}^{(x,y)}$ in this region in the form ($i\varepsilon_n \sim T \ll \mu$)

$$G^{(x,y)} = \frac{iB_z^* v\delta_y}{(i\varepsilon_n - u)(\varepsilon_1 - \varepsilon_2)((v\delta_y)^2 + 4|B_z|^2)} \begin{Vmatrix} \mu + iv\delta_x & \mu + iv\delta_x \\ \mu - iv\delta_x & \mu - iv\delta_x \end{Vmatrix}. \quad (A.2)$$

The velocity $|v|$ figuring in the integral $\oint dS/|v|$ is, according to (4), equal to

$$|v| \approx |v_x| = \left|\frac{\partial \varepsilon}{\partial p_x}\right| = \frac{v\delta_y}{[(v\delta_y)^2 + 4|B_z|^2]^{1/2}} \approx \frac{v\delta_y}{2|B_z|}$$

which leads to a logarithmic integration over the region $B^{3/2}/v \ll v\delta_y \ll B$. It is convenient to write the matrix in (A.2) in the form

$$\mu(\hat{e} + \hat{\tau}_x) + iv\delta_x(\hat{\tau}_z - i\hat{\tau}_y).$$

As a result, it is easy to separate out the logarithmic contribution to the coupling coefficients for the equation depicted by Fig. 2 (i.e., the expression (7)) if we write the equation as follows:

$$RX\pi^{-2}(\alpha_s^{(\nu)} + \beta_s^{(\nu)})(k_1\hat{e} + k_2\hat{\tau}_x), \quad (A.3)$$

where

$$k_1 = \ln\left(\frac{T^*}{\Delta E}c_1\right)\left(\frac{T^*}{\Delta E}\right)^{1/2}, \quad k_2 = -\ln\left(\frac{T^*}{\Delta E}c_2\right)\left(\frac{T^*}{\Delta E}\right)^{1/2} \quad (A.3')$$

Here $\ln c_1$ and $\ln c_2$ are not small, but the estimation of them requires a numerical integration. Similar computations lead to the following expressions connecting the superconducting gaps in the x and z directions:

$$RX\pi^{-2}(\alpha_s^{(z)} - \beta_s^{(z)})(k_1\hat{e} - k_2\hat{\tau}_z).$$

[1)] In[9] the controlling parameter of the transition is assumed to be the tetragonal distortion.

[2)] Below μ is measured from thispoint.

[3)] A similar problem has been considered[6] in the Labbe-Friedel model for systems of three weakly-coupled filaments. Above we have shown that the filaments are strongly coupled. An anisotropy in H_{c2} (see[16]) could arise only in the case of severe uniaxial distortions.

[4)] In[9] there is an arithmetical error in the sstimation of d_1. Together with the estimate from the x-ray data of[18] with the aid of Eq. (26) of[9] we find d_1 to lie within the limits $1-1.5$ eV.

[5)] For $\Theta \sim 200$ K, $T_e \sim 20$, and $T^* \sim 600$ K in (25), we have $P(X) \sim 27$ and $R \sim 0.37$.

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