Contribution to the theory of the properties of the superconductors with β-W structure

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A theory of the properties of the superconductors with β-W structure is proposed on the basis of the assumption that in linear chains the Fermi level passes through the reciprocal-lattice point X, where the conduction bands are twofold degenerate and possess a linear dispersion law. It is shown that in this case the electronic corrections to the energy induce a structural transition that precedes the transition to the superconducting state. The two transitions should, however, occur at close temperatures. This solves the problem of the connection between instability and superconductivity in these compounds as two aspects of the same phenomenon, namely, instability of the electron spectrum. The theory predicts logarithmic temperature dependences for all the quantities above the transition point. For the elastic moduli in the high-temperature region, in particular, these dependences are linear, as borne out by experiment.

1. INTRODUCTION AND FORMULATION OF THE PROBLEM

Superconductors of the type Nb_3Sn have now been quite thoroughly studied. Numerous experimental data are given in Testardi's review article [1]. The principal difference between the properties of this "high-temperature" group of compounds and those of the normal superconductors is the dependence on temperature of the various characteristics above the transition point T_c. As noted by Testardi, the most distinctive feature is the correlation with the structural transition. For good samples, the latter transition occurs at temperatures T_m which are higher than T_c. If the structural transition does not occur, then a tendency toward it is observed which is manifested in the softening of the elastic moduli. In all the known cases T_m differs from T_c by not more than a factor of two, whereas the temperature dependences presaging the transition extend to temperatures of 300–400 K. The behavior of the magnetic susceptibility, as well as of the Knight shift, varies from compound to compound.

Weger[2] was apparently the first to point out that, on account of a small overlap of the d shells, the three systems of linear arrays of transition-element atoms could play an important role in the properties of the β-W structure. This agrees qualitatively with the more critical behavior of all the properties when transition-element atoms are introduced into the T_3X structure.[1] The tight-binding approximation for the d electrons in a chain has figured in all the theoretical papers[3–5], where an unusually large and narrow peak is postulated in one form or another to exist in the density of states in the vicinity of the Fermi energy. This is most consistently done in Labbe and Friedel's papers[4], where the indicated peak in the density of states $\nu(\epsilon)$ arises as a result of the assumption that the Fermi level lies close to the empty d band at $k=0$ (the point Γ), since in the one-dimensional band $\nu(\epsilon)\propto\epsilon^{-1/2}$ as $\epsilon\to 0$.

Weger[6] has discussed the possibility of the appearance of a similar peculiarity at the point X of the reciprocal lattice after the structural transition as a mechanism by which the density of states and, consequently, T_c, could rise. Finally, let us recall that the three orthogonal systems of chains have been investigated by Barišic and DeGennes[7] and Weger[8]—although as macroscopically one-dimensional objects—for the purpose of explaining the nature of the anisotropy in the upper critical fields[7] and of interpreting the above-indicated temperature dependences in the magnetic properties in the language of fluctuation phenomena.[8]

Although it is possible in the Labbe-Friedel theory[4] to account for the structural transition by an appropriate choice of the constants, this is achieved by locating the Fermi level very close to the bottom of the d band (10^{-3}–10^{-2} eV). The proximity of the transition temperatures T_m and T_c is not a basic feature of the model.

If the electrons in the chains are indeed localized, then from the point of view of the Luttinger theorem[9] on the filling up of bands, the condition for the total population of the d band of an individual chain will be the location of the chemical potential at the extreme point, since there are two transition-element atoms per lattice period along a chain in the A-15 structure. Consequently, it is natural to locate the Fermi level at the point X of the reciprocal lattice. Below we assume just this situation. It turns out that all the properties of the superconductors with the β-W structure can be explained as the result of the instability of the electron spectrum at the point X against the electron-lattice and electron-electron interactions. The nature of this instability is connected with the twofold degeneracy of the levels at the point X and with the linear dispersion law in its vicinity. Therefore, the instability of such a spectrum is related to the instability of the spectrum of the one-dimensional metal discovered by Bychkov, Dzyaloshinskiĭ, and this author in [10], where it is shown that the characteristic feature of the one-dimensionality is the connection between the Cooper pairing and the Peierls doubling of the lattice period.[1)]

The circumstance suggesting the application of the ideas put forward in [10] is the logarithmic dependence of the elastic moduli in the region of fairly high temperatures [1]:

$$C_{ij}=A+B\ln T.$$

The doubling of the period in the individual chains of Nb atoms has indeed been observed to occur in the structural transition in Nb_3Sn by Shirane and Axe [12]. Since there are two transition-element atoms per β-W lattice period in a chain, the logarithmic corrections to the phonon frequencies which were found in [10] pertain to phonons with the wave vector $q=0$. It will be shown below that the Cooper pairing is also connected with the tetragonal deformation in the β-W structure, the structural transition in a pure sample preceding the superconducting transition.

In the one-dimensional case, in contrast to the BCS model of the theory of superconductivity, it is not possible even in the limit of weak interactions to obtain closed formulas describing the vicinity of the transition point. The result of the theory expounded in [10,11] consists in the assertion that

$$T_m \sim T_c \sim \tilde{\omega} \exp(-1/|g_1|), \tag{1}$$

where $\tilde{\omega}$ is a characteristic cutoff energy, which is, generally speaking, of the order of the Debye frequency, and g_1 is the effective dimensionless constant of the interelectron attraction. In consequence, T_m and T_c are determined only up to a constant factor.

It is known from experiment [1] that for

	Θ_D, °K	T_m, °K	T_c, °K
V_3Si:	500	18÷25	17
Nb_3Sn:	300	43	18.2

According to (1), $|g_1| \sim \ln^{-1}(\Theta_D/T)$ and, consequently, the electron-electron interactions are not too weak. The situation for V_3Si is apparently more favorable.

In Sec. 2 we shall find the temperature dependences of the physical quantities in the region of fairly high temperatures. The contribution from the electron interactions to, for example, the structure quantities turns out to be significant in the vicinity of the transition point, and is investigated in Sec. 3. The comparison of the conclusions of the theory with the experimental situation is carried out in the course of the exposition. Finally, in Sec. 4 we demonstrate the overall self-consistency of the conclusions of the theory. We also discuss in this section the specific connection between structural instability and superconductivity in quasi-unidimensional systems, thereby demonstrating that from the point of view of the proposed theory quasi-unidimensional systems which become structurally unstable at sufficiently high temperatures are potential objects on the basis of which higher superconducting-transition temperatures can be realized.

2. THE CHARACTERISTICS OF THE ELECTRON SPECTRUM. THE BEHAVIOR OF THE PHYSICAL QUANTITIES IN THE HIGH-TEMPERATURE REGION

Compounds of the type Nb_3Sn have the O_h^3 space group. The reciprocal lattice is a primitive cubic lattice. The groups of the wave vectors at the points of symmetry and the matrices of the generating elements of the little groups have been constructed by Gorzkowski [13]. The characters of the representations at the points Γ and X have been found by Weger [6]. For the reasons indicated above, we shall be interested in the electron spectrum in the vicinity of the point X and in the dependence of this spectrum on strain and magnetic field.

Figure 1 shows the symmetry possessed by the individual linear chains of transition-element atoms along the z axis in the crystalline surroundings. Supposing that in the first approximation the d electrons are localized on one chain, we shall assume that all the quasi-momentum-component dependences in the $\{p_x, p_y\}$ plane which characterize the electron spectrum at the point X are extra small, owing to the weakness of the interchain transition. Therefore, in the first approximation, the spectrum is planar.

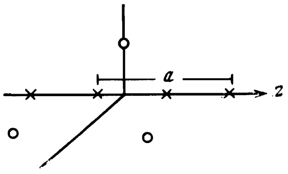

FIG. 1

The little co-group (the direction group) of the point X is the point group D_{4h}, but the group of the **k** vector contains a rotation through $\pi/2$ followed by a nontrivial translation by $a/2$, where a is the period of the chain. As noted in [6], this circumstance leads to an inevitable twofold degeneracy of the levels at the point X. As we shall see presently, among the four representations X_i (i = 1, ..., 4) two, X_2 and X_4, allow, without allowance for spin, a finite value for the electron velocity at the point $p_z = 0$.$^{2)}$ In Table I, we list the elements of the finite group of the point X in standard notation (see for example, [14,15]), as well as the characters of the representations. It is not difficult to verify that this group differs from the group of the **k** vector of the point X of the reciprocal diamond lattice only in the orientation of the nontrivial elements with respect to the principal axes of the crystal: the congruence is attained by rotating the x and y axes through 45° about the z axis.

To find the electron spectrum in the vicinity of the point X, the representation product $X_i^* \cdot X_i$ should be expanded in terms of the representations of the point group D_{4h}. Since $D_{4h} = D_4 \otimes C_i$, it is convenient to specify the latter by the representations of the group D_4, which are even or odd under inversion. The products $X_i^* \cdot X_i$, as is easy to verify, contain the following representations:

$$\begin{gathered} X_1^* \cdot X_1, \quad X_3^* \cdot X_3: \quad B_1^-, \quad A_1^+ + A_1^- + B_1^+; \\ X_2^* \cdot X_2, \quad X_4^* \cdot X_4: \quad A_2^-, \quad A_1^+ + B_1^+ + B_2^-. \end{gathered} \tag{2}$$

Here B_1^- and A_2^- change sign under time inversion (antisymmetrized products). The remaining representations can enter into the electronic Hamiltonian only together with quantities that are invariant under time reversal.

TABLE I

[14]	[15]	X_1	X_2	X_3	X_4
E	e	2	2	2	2
Tm_y	$(\tau\|c_4)$	0	0	0	0
C_2	$(0\|c_4^2)$	−2	2	−2	2
Tm_z	$(\tau\|c_4^3)$	0	0	0	0
C_2'	$(0\|u_2)$	2	0	−2	0
Tm_x	$(\tau\|c_4u_2)$	0	0	0	0
C_2''	$(0\|c_4^2u_2)$	−2	0	2	0
TI	$(\tau\|c_4^3u_2)$	0	0	0	0
I	$(0\|i)$	0	0	0	0
TC_2''	$(\tau\|ic_4)$	0	0	0	0
m_x	$(0\|ic_4^2)$	0	0	0	0
TC_2'	$(\tau\|ic_4^3)$	0	0	0	0
m_z	$(0\|iu_2)$	0	2	0	−2
TC_2	$(\tau\|ic_4u_2)$	0	0	0	0
m_y	$(0\|ic_4^2u_2)$	0	2	0	−2
T^y	$(\tau\|ic_4^3u_2)$	0	0	0	0

TABLE II

$t \to -t$ change sign	$t \to -t$ invariant	Quantities entering into the products $X_i^* \cdot X_i$
	A_1^+	$p_x^2 + p_y^2$; p_z^2; ε_{zz}; $\varepsilon_{xx} + \varepsilon_{yy}$; $p_xp_y\varepsilon_{xy}$; $\sigma\mathbf{H}$; $\sigma_xH_x + \sigma_yH_y$
	A_1^-	σ_zp_z; p_zH_z
	B_1^+	$p_x^2 - p_y^2$; $\varepsilon_{xx} - \varepsilon_{yy}$; $\sigma_xH_x - \sigma_yH_y$; u_z
	B_2^-	$p_xH_y + p_yH_x$; $\sigma_zp_z\varepsilon_{xy}$; $(p_x\sigma_x + p_y\sigma_y)\,\varepsilon_{xy}$; $\sigma_z(p_x\varepsilon_{yz} + p_y\varepsilon_{xz})$
A_2^-		p_z; $p_x\varepsilon_{xz} + p_y\varepsilon_{yz}$
B_1^-		$p_z\varepsilon_{xy}$

In Table II we list the various quantities for the representations that enter into the products $X_i^* \cdot X_i$. Using the method of invariants [15], and introducing the Pauli matrices τ_x, τ_y, and τ_z, we can write the Hamiltonian for the electrons in the vicinity of the point X as follows:

$$\hat{\varepsilon}(p)=\hat{e}A_{1+}+\hat{\tau}_z A_2^- +\hat{\tau}_x B_1^+ +\hat{\tau}_y B_2^- \quad (X_2,\ X_4), \tag{3}$$

where A_1^+, A_2^-, B_1^+, and B_2^- contain, generally speaking, all the combinations that can be formed from the quasi-momentum components and the external influences transforming according to the corresponding representation. Above we considered the single-valued representations; therefore, the combinations in Table II that contain the spin matrices (with the exception of the term σH) owe their origin to the spin-orbit interaction, i.e., they are of relativistic smallness. In the compounds under consideration, the spin-orbit interaction is not too small. As to those terms containing the quasi-momentum components p_x and p_y, we shall assume they are smaller than the rest, since the interchain coupling is considered to be weak.

Thus, according to (2) and Table II, the electron energy has the form

$$\hat{\varepsilon}(p_z)=ap_z^2\hat{e}+vp_z\hat{\tau}_z. \tag{4}$$

In the presence of a strain ϵ_{ik}, the correction to the electron energy in the representation of second quantization has the form $\lambda\psi^+(A\epsilon)\psi$. For the correction to the thermodynamic potential Ω, we have

$$\frac{\delta\Omega}{\delta\lambda}=\langle\psi^+(A\varepsilon)\psi\rangle.$$

This expression can be rewritten in terms of the quantities of field theory: the Green functions G(p) and the vertex part $\mathscr{T}(p_1, p_2, p_3, p_4)$. The quadratic–in the strain–correction to the elastic energy due to the electrons and including the electron-electron interaction can be written as follows [16]:

$$\delta F=\frac{1}{2}(A\varepsilon)_{\alpha\beta}{}^{ik}(A\varepsilon)_{\beta\alpha}{}^{ki}\int G^{(i)}(p)G^{(k)}(p)\,dp$$
$$+\frac{1}{2}(A\varepsilon)_{\alpha\gamma}{}^{ik}\iint G^{(i)}(p)G^{(k)}(p)\mathscr{T}^{ilkm}_{\alpha\beta\gamma\delta}G^{(l)}(p')G^{(m)}(p')\,(A\varepsilon)_{\beta\delta}{}^{lm}dp\,dp'. \tag{5}$$

The expression (5) is diagrammatically represented in Fig. 2. Here the Greek indices indicate summation over the spin variables, while the Latin indices number the bands:

$$\int dp=T(2\pi\hbar)^{-1}\sum_{\omega}\int dp_z.$$

In the vicinity of the Fermi surface, the Green functions take the form

$$G^{(k)}(p)=a^{(k)}(i\omega_n-\varepsilon_k(p))^{-1}, \tag{6}$$

where $a^k \leq 1$.

Only the temperature-dependent terms in (5) have any physical meaning. We shall see in the next section that the contribution from the second term in (6) is of the order of $g_1 \ln(\tilde{\omega}/T)$ at high temperatures; therefore, this term is, as was asserted at the beginning of the paper, assumed to be small.

Thus, at high temperatures, we shall consider the contribution from the simple loop in Fig. 2. The dependence on temperature arises only if by change the indices i and k in the first term in (5) belong to different bands: $\epsilon_{1,2} = \pm vp_z$. In fact,

$$\int G^{(1)}G^{(2)}\,dp \propto \int \operatorname{th}\frac{vp_z}{2T}\frac{dp_z}{vp_z} \propto \frac{1}{v}\ln\frac{\tilde{\omega}}{T}.$$

According to Table II, the off-diagonal elements in the Hamiltonian are of the form

$$\hat{\tau}_x[D_1(\varepsilon_{xx}-\varepsilon_{yy})+D_2u_z],$$

where u_z is the "sublattice" displacement, e.g., the relative displacement of every other transition-element atom in the chain.

The strain contribution to the first term of (5) made by the system of chains along the [001] direction per unit volume will be

$$\delta F_z=-\frac{D_1^2}{2a^2\pi v}(\varepsilon_{xx}-\varepsilon_{yy})^2\ln\frac{\tilde{\omega}}{T} \tag{7}$$

(a is the lattice constant and $\tilde{\omega}$ is the cutoff energy).

Summing over all the orthogonal chains, we obtain

$$\delta C_{11}=-\frac{2D_1^2}{a^2\pi v}\ln\frac{\tilde{\omega}}{T}, \quad \delta C_{12}=\frac{D_1^2}{a^2\pi v}\ln\frac{\tilde{\omega}}{T}. \tag{8}$$

Allowance for the interaction terms becomes essential when $g_1 \ln(\tilde{\omega}/T) \sim 1$. Jumping ahead, we note that these terms always increase the magnitude (8) of the effect without changing the relative sign for δC_{11} and δC_{12}. Since u_z and $\epsilon_{xx}-\epsilon_{yy}$ belong to the same representation, there also occurs, according to (5), a logarithmic shift in the optical frequency corresponding to the vibrations of the atoms of the chain relative to each other.

In the above-considered approximation, the modulus C_{44} is temperature independent.3) The experimental data [1] indicate that the modulus C_{44} also decreases with decreasing temperature, although the magnitude of the effect is markedly smaller than, for example, for C_{11}. Thus, the change in C_{44} from 300 to 100 K in V_3Si is roughly ten times smaller than for C_{11}; in Nb_3Sn, the change in C_{44} is smaller than the change in C_{11} by a factor of four to five. It can be seen from Table II that the off-diagonal components of the strain tensor, which lead to the logarithmic temperature dependences in the simple loop in Fig. 2, are due, in the self-consistent field approximation, only to the terms containing the interchain electron transitions (besides the extra smallness owing to the spin-orbit coupling).

The experimental data indicate that the logarithmic behavior of all the quantities is valid up to a temperature of the order of the transition temperature $T_m \sim 10^2$ K. If the interchain electron transitions are attributed to some interaction V_{12},4) then the distortion of the initial plane spectrum is characterized by the energy V_{12}^2/E_F. The condition that this distortion be insignificant right up to temperatures of order 10^2 K yields the estimate

$$V_{12}/E_F \leqslant (T_m/E_F)^{1/2} \sim 10^{-1}.$$

Such an estimate does not seem to be too optimistic, and is obtained even in the strong-coupling models (see [6]) without allowance for the inhibitory effects of the crystalline surroundings.

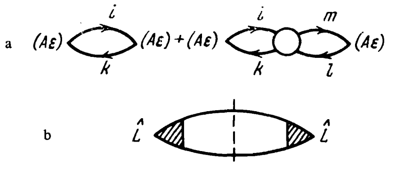

FIG. 2

According to (8), the slope of the ln T dependence of C_{11} is twice as large as for C_{12}. It is too early to speak of any quantitative agreement of the experimental data with this symmetry effect, although the qualitative picture is correct [1].

The majority of the data on the elastic moduli were taken from velocity-of-sound measurements [1]. The static measurements of the elastic moduli have a large scatter and, in our opinion, are in poor agreement with the ultrasound data. In this connection, let us point out that the proposed theory predicts the dispersion of the elastic moduli at wave vectors $q \sim T/v$. This dispersion leads to a situation in which for the acoustic vibrations with

$$\frac{\pi}{a} \gg q \gg q^* = \frac{T}{v} \sim \frac{10^{-2}}{a}$$

the temperature variations in the elastic moduli computed from the velocity of sound can turn out to be considerably smaller than the corresponding quantities obtained in the static measurements. The dispersion law for the acoustic vibrations is not linear and contains logarithmic q dependences.

Let us, for example, consider sound propagating along the z axis. To it corresponds a z dependence of ϵ_{yy} and ϵ_{xx} of the form $\exp(iq_z z)$. Therefore, we must find the contribution to the elastic vibrational energy (5) made by the system of chains along the [001] direction in the form:

$$\delta F_z(q_z) \infty (\varepsilon_{xx}(q_z) - \varepsilon_{yy}(q_z))^2 \int G^{(1)}(p) G^{(2)}(p - q_z)\, dp.$$

We find after the calculations that the expression (5), with allowance for the finite magnitude of the component $q_z \ll \pi/a$, can be written in the form

$$\begin{gathered} \delta F_z(q_z) = -\frac{D_1^2}{2a^2\pi v}(\varepsilon_{yy} - \varepsilon_{xx})^2 \left\{ \ln\frac{\tilde{\omega}}{T} + U(q_z) \right\}, \\ U(q_z) = \psi\left(\frac{1}{2}\right) - \frac{1}{2}\left[\psi\left(\frac{1}{2} + \frac{ivq_z}{4\pi T}\right) + \psi\left(\frac{1}{2} - \frac{ivq_z}{4\pi T}\right)\right], \end{gathered} \tag{9}$$

where ψ is the derivative of the logarithm of the gamma function. The asymptotic expressions for U(x) have the form

$$U(x) = \begin{cases} -{}^7/_2\zeta(3)x^2, & x \ll 1 \\ -\ln x, & x \gg 1 \end{cases}. \tag{9'}$$

Let **q** be arbitrarily oriented: $\mathbf{q} = \{q_x, q_y, q_z\}$. Each component q_i figures only in the expression for δF connected with the contribution from the chains that are parallel to it. Summing over all the chains, we obtain

$$\begin{gathered} \delta F(\mathbf{q}) = -\frac{D_1^2}{2a^2\pi v}\left\{ \varepsilon_{xx}^2\left(2\ln\frac{\tilde{\omega}}{T} + U(q_y) + U(q_z)\right) \right. \\ + \varepsilon_{yy}^2\left(2\ln\frac{\tilde{\omega}}{T} + U(q_x) + U(q_z)\right) + \varepsilon_{zz}^2\left(2\ln\frac{\tilde{\omega}}{T} + U(q_x) + U(q_y)\right) \\ \left. -2\varepsilon_{xx}\varepsilon_{yy}\left(\ln\frac{\tilde{\omega}}{T} + U(q_z)\right) - 2\varepsilon_{yy}\varepsilon_{zz}\left(\ln\frac{\tilde{\omega}}{T} + U(q_x)\right) - 2\varepsilon_{xx}\varepsilon_{zz}\left(\ln\frac{\tilde{\omega}}{T} + U(q_y)\right)\right\}. \end{gathered} \tag{10}$$

For the transverse sound, $\mathbf{q} \parallel [110]$ (vibrations in the same plane), the ultrasound measurements yield the modulus $C_S = {}^1/_2(C_{11} - C_{12})$. We have

$$\delta C_s(\mathbf{q}) = -\frac{D_1^2}{2a^2\pi v}\left\{3\ln\frac{\tilde{\omega}}{T} + \frac{1}{2}U\left(\frac{|q|v}{\sqrt{2}\,4\pi T}\right)\right\}. \tag{11}$$

For $vq/\pi T \gg 1$, we find, according to (9′), that

$$\frac{1}{2}\delta(C_{11} - C_{12}) = -\frac{D_1^2}{2a^2\pi v}\left\{3\ln\frac{\tilde{\omega}}{T} - \frac{1}{2}\ln\left(\frac{qv}{\sqrt{2}\,4\pi T}\right)\right\}. \tag{11'}$$

The neutron-scattering measurements of the phonon spectra (see [1]) indicate a distortion of the acoustic dispersion law, but these data are at present insufficient for comparison with (10) and (11′). This dispersion apparently explains the above-indicated noncoincidence of the slopes of ${}^1/_2C_{11}$ and $-C_{12}$.

Let us proceed to discuss the magnetic susceptibility and the Knight shift. If the Knight shift is due to the d electrons, then the sign of the effect is not uniquely connected with the sign of the magnetic susceptibility. We can only state from Fig. 3 that the dependence of both quantities, for example in V_3Si, on ln T is linear at high temperatures.

The quadratic—in the magnetic field—correction to the free energy can easily be obtained from (5) by replacing in this formula $\hat{A}\hat{\epsilon}$ by the corresponding matrix elements from Table II that are proportional to the field H. The term $\boldsymbol{\sigma}\mathbf{H}$ does not contain transitions from 1 to 2 and gives the paramagnetic contribution from the d electrons. The corrections to χ_{par} due to the interaction were computed for the one-dimensional chain in [11]; this result remains valid for the structure under consideration if the interaction with the s electrons is neglected. The corresponding contribution in the high-temperature region is

$$\frac{\delta\chi_{par}}{\chi_{par}} \sim -\frac{1}{2}g_1^2\ln\frac{\tilde{\omega}}{T}.$$

In an expression of the type (5), the logarithmic contribution in the simple loop for the free energy is given by the representations $B_1^+(\sigma_x H_x - \sigma_y H_y)$ and $B_2^-(p_x H_y + p_y H_x)$. Both terms lead to a paramaramagnetic contribution to the susceptibility that increases with decreasing temperature as ln T. As to the second combination, it is responsible for the Van Vleck paramagnetism, but the contribution from it should be considered to be small. The smallness, which is connected with the representation B_1^+, is due to the spin-orbit interaction.

Thus, contained in the ln T dependence of the magnetic susceptibility at high temperatures are two competing paramagnetic contributions: increasing and decreasing. It can be seen from Fig. 3, however, that the change in the susceptibility for V_3Si is by no means small and most likely cannot be due to the contribution from a term that is quadratic in the spin-orbit interaction. Furthermore, it seems that the experimental curves for both the susceptibility and the temperature dependence of the elastic moduli exhibit a certain tendency toward saturation in about the 300-400-K range.[1] This circumstance makes it necessary to discuss the possibilities connected with another choice of terms at the point X.

The representations X_2 and X_4 are a natural generalization of the terms of the linear one-dimensional

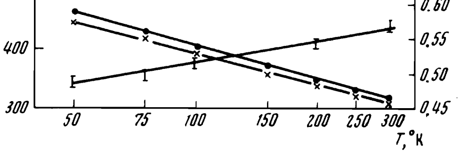

FIG. 3. The dependence of the magnetic susceptibility χ and the Knight shift K_V on *l*nT in V_3Si. For χ, the results of [17] were used (the points ● and X correspond to different samples), and the data on the Knight shift were taken from [1].

chain, which has been considered earlier [10,11], and go over into the latter when the crystalline surroundings are neglected. The representations X_1 and X_3 have zero slope when spin is neglected and go over, as we move away from the point X, into the twofold degenerate representation Δ_5. Therefore, these bands are either completely filled or completely empty, which excludes the concept of d-electron conduction. Still another possibility, which is compatible with Luttinger's theorem [9], is to assume that this band is one-quarter or half filled. However, in this case all the distinctive features which were the subject of the discussion above will pertain to transitions with a doubling or a quadrupling of the period of the A-15 structure.

Allowance for spin leads to the splitting of the X_2 and X_4 terms. We can write in accordance with (2) and Table II:

$$\hat{\varepsilon}(p)=\tilde{v}\hat{\tau}_z\sigma_z p_z+\hat{\tau}_x B_1{}^+ +\hat{\tau}_y B_1{}^-.$$

Thus, the functions $\{\psi_{1\uparrow}, \psi_{2\downarrow}\}$ form the twofold degenerate term $\epsilon_1(p)=\tilde{v}p_z$, while the functions $\{\psi_{1\downarrow}, \psi_{2\uparrow}\}$ produce the term $\epsilon_2(p)=-\tilde{v}p_z$. Therefore, if the Fermi level passes through the point X, then the spin-orbit interaction can lead to the appearance of a small number of electrons or holes. The volume of these "pockets" corresponds to

$$p_z^*\sim\frac{\tilde{v}}{v}\frac{2\pi}{a}\sim\frac{V_{so}}{E_F}\frac{2\pi}{a}.$$

The representation B_1^+, which contains $\epsilon_{xx}-\epsilon_{yy}$, leads again to expressions of the form (8) and (10), with the difference that the velocity $\tilde{v}$ is of relativistic smallness, while the cutoff energy is of the order of V_{s0}. It is reasonable to assume for the magnitude D_1 of the deformation potential of the d electrons the values $D_1\sim 1-3$ eV; $\delta C_{11}\sim\delta C_{12}\sim 10^{12}$ erg/cm^3. From this we obtain the extimate $\tilde{v}\sim 10^7$ cm/sec, i.e., $V_{s0}/E_F\sim 10^{-1}$.

In contrast to the first case for these terms, the same objections which were discussed in connection with the Labbe-Friedel model can be advanced against the location of the chemical potential at the point of degeneracy. The requirement that a detached small portion of the carriers should cross over to the s band is artificial and can be discussed only if there are experimental indications to this. We consider it necessary to note this possibility in connection with the results of [17] for the susceptibility χ in V_3Si (Fig. 3). The large magnitude of the susceptibility itself and its variation in the 300–50-K interval could be attributed to the X_2 or X_4 term. In fact, the standard term $\mu_B\sigma H$ in the Hamiltonian has off-diagonal transitions over the bands $\epsilon_{1,2}=\pm\tilde{v}p_z$ if the field H is perpendicular to the chain in question. Summing over the two possible systems of chains, we obtain the temperature-dependent term in (5):

$$\delta F=-\frac{e^2\hbar^2H^2}{8\pi m^2c^2a^2\tilde{v}}\ln\frac{V_{so}}{T}.$$

Another possible explanation of $\delta\chi_{par}$ is connected with the electron interaction (see the following section).

To conclude this section, let us discuss briefly the temperature dependence of the resistance and of the coefficient of thermal expansion. In Figs. 4 and 5 we have plotted the resistance for different A-15 compounds as a function of lnT (the data were taken from Testardi's review article [11]). There is practically no evidence of the standard law $\rho\sim T$. This in itself is not surprising, since the conductivity along the linear chain in the presence of impurities has a special character owing to the quasi-localization of the electrons. Even the best samples of the A-15 compounds are fairly contaminated on account of internal strains, inhomogeneities, etc. The effective mean free path l can be estimated from the observation that different samples of V_3Si or Nb_3Sn prepared by the same method can either exhibit or not exhibit a structural transformation. As can be seen from the results of the following section, this depends on the relation between l and the correlation length ξ_0, for which we take the expression from the BCS theory (see (11)):

$$\xi_0=\hbar v/2\pi T_m.$$

Setting $v\sim 10^7$ cm/sec and $T_m = 40$ K, we obtain $l\sim 10^{-6}$ cm. As to the linear dependence of ρ on lnT in Figs. 4 and 5 in the region $T\gg T_m$, not having the theoretical formulas, we can only state the fact that the electron-phonon and electron-electron scattering amplitudes contain, according to the results of the following section, logarithmic terms.

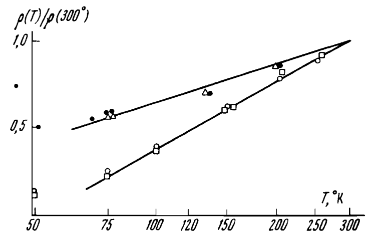

FIG. 4. The resistance ratio $\rho(T)/\rho(300\ ^\circ K)$ for different compounds as a function of lnT (data taken from [1]): ○–V_3Ge, □–V_3Si, ●–V_3Ga, and Δ–V_3Sn.

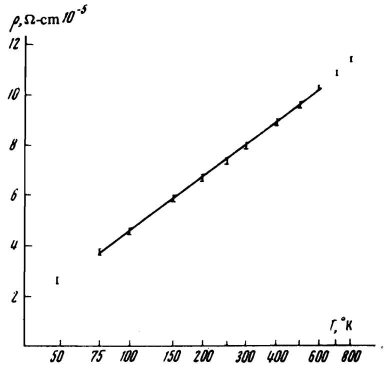

FIG. 5. Resistance in Nb_3Sn as a function of lnT (constructed from curves in [1]).

Let us finally touch upon the question of the coefficient of thermal expansion. The dependence of the electron terms on strain, together with the quadratic strain dependences, leads to the appearance in the free energy of terms linear in ϵ_{ii}, with temperature-dependent parts in the form

$$\varepsilon_{ii}\sum_k a_k n_k(T)=AT^2\varepsilon_{ii},$$

where $n_k\propto T^2$ is the number of carriers in the k-th band. Minimizing the free energy with respect to ϵ_{ii}, we find for the lattice-parameter temperature dependence due to the electronic contribution the expression

$$\varepsilon_{ii}=-\frac{AT^2}{C_{11}+2C_{12}}. \qquad (12)$$

In Testardi's work [18], the coefficient of thermal expansion α in V_3Si and V_3Ge is interpolated as $\alpha \propto \ln T$. Analysis of these data [18] shows that α can equally well be described by a linear dependence on T.

3. ALLOWANCE FOR THE ELECTRON-ELECTRON INTERACTION. INSTABILITY AND SUPERCONDUCTIVITY

The nature of the electronic corrections to the free energy leads to a structural transition to the tetragonal phase. The electron-electron interactions considered in [10,11] give rise to other distinctive features, in particular, of the Cooper-pairing type. We obtain the correlation between these transitions by taking into account in (5) the second term containing the effects of the electron interaction. We stipulate at once that we restrict ourselves to the parquet approximation, i.e., we assume the interactions to be weak. In general, the temperature range where the dependence of the various quantities on $\ln T$ is linear is fairly wide. We shall assume that the three-dimensionality effects (the interchain interaction) are characterized by the smallest constants.

The definition of the vertex part $\mathscr{T}_{\alpha\beta\gamma\delta}(p_1, p_2, p_3, p_4)$ as the Fourier component of $\langle T(\psi_\alpha(1)\psi_\beta(2)\psi_\gamma^+(3)\psi_\delta^+(4))\rangle$ is well known:

$$\begin{gathered}\langle T(\psi_\alpha(1)\psi_\beta(2)\psi_\gamma^+(3)\psi_\delta^+(4))\rangle \\ \Rightarrow -G_{\alpha\gamma}(p_1)G_{\beta\delta}(p_2)+G_{\alpha\delta}(p_1)G_{\gamma\beta}(p_2) \\ +G_{\alpha\zeta}(p_1)G_{\beta\eta}(p_2)\mathscr{T}_{\zeta\eta\tau\nu}(p_1,p_2,p_3,p_4)G_{\tau\gamma}(p_3)G_{\nu\delta}(p_4).\end{gathered} \tag{13}$$

(We have not written out the conservation laws.) Let us briefly explain the changes introduced by the crystal symmetry. In the absence of external fields and interactions (except those which are assumed to be included in the self-consistent field), the vicinity of the point X corresponds to two bands: $\epsilon_{1,2} = \pm\tilde{v}p_z$. The interactions themselves are short-range, but the invariance of (13) imposes definite limitations on the interband transitions. If we choose the representation D_X for the wave functions, then, say, the pair $\psi_{(1)}\psi^+_{(3)}$ corresponds to the decomposition of $D_X^* \otimes D_X$ into the four irreducible representations of the point group of the point X:

$$D_X^*\otimes D_X = A_0 + A_z + A_x + A_y,$$

where the representations A_0 and A_Z are diagonal in some basis corresponding to the levels $\epsilon_{1,2}(p)$ near X. In the preceding section we associated in the matrix Hamiltonian the 2×2 matrices $\hat{e}$, $\hat{\tau}_x$, $\hat{\tau}_y$, and $\hat{\tau}_z$ with all the representations. Therefore, to any diagram in which the electron line from 1 terminates at 3, and the one from 2 terminates at 4, will correspond the contribution to $\mathscr{T}$ given by

$$(g_0\hat{e}\cdot\hat{e} + g_z\hat{\tau}_z\cdot\hat{\tau}_z + g_x\hat{\tau}_x\cdot\hat{\tau}_x + g_y\hat{\tau}_y\cdot\hat{\tau}_y)\,\delta_{\alpha\gamma}\delta_{\beta\delta}. \tag{14}$$

We choose the expression (14) as the bare interaction. It is easy to see that only interband transitions of the type (11; 22), (12; 21), (12; 12) are different from zero. The diagonal transitions (11; 11) make no contribution to the parquet equations. If the systems studied in [10,11] are considered in a doubled lattice, then a correspondence can be established between the vertices figuring in both cases. Thus, it turns out, in particular, that the transition (11; 22) corresponds to the momentum-transferring vertex $\mathscr{T}_{+\!+\!-\,-}$ introduced in [11]. The correspondence between the bare constants of [11] and (14) is as follows:

$$g_1 = g_x + g_y;\quad g_2 = g_0 + g_z;\quad g_3 = g_x - g_y. \tag{15}$$

Generally speaking, there are no grounds for neglecting in (14) and (15) the dependence on the angles between the momenta. For a plane spectrum, only the orientation of p_z remains. The notation

$$\mathscr{T}^{1221}_{\alpha\beta\gamma\delta} = \gamma_1\delta_{\alpha\gamma}\delta_{\beta\delta} - \gamma_2\delta_{\alpha\delta}\delta_{\beta\gamma};$$

$$\mathscr{T}^{1122}_{\alpha\beta\gamma\delta} = \gamma_3(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})$$

allows us to directly use the results obtained by Dzyaloshinskiĭ and Larkin in [11], since the parquet equations for both cases have the same solutions. The difference in the physical interpretation consists, as has already been indicated, in the fact that in the one-dimensional model of [10,11] a structural transition corresponds to a doubling of the period, whereas the distinctive features in the β-W structure pertain to the wave vector $q = 0$.

It is convenient to compute the complete expression (5) by Sudakov's method. Figure 2b shows a diagrammatic representation of the corresponding procedure, which was used earlier in [11]. The dashed line indicates the cross section where the logarithmic variable has its maximum value, i.e., where the running integration momentum is nearest to the Fermi point. For the hatched triangles, which we denoted by L and which depend on the nature of the quantities being averaged, we obtain the equations[5)]

$$L_{\delta\rho}{}^{21}(\xi) = L_{\delta\rho}^{(0)21} - \frac{1}{2}\int_0^\xi \gamma_3 d\xi\,(L_{\nu\nu}{}^{12}\delta_{\rho\delta} - L_{\delta\rho}{}^{12})$$

$$-\frac{1}{2}\int_0^\xi (\gamma_1 L_{\nu\nu}{}^{21}\delta_{\rho\delta} - \gamma_2 L_{\delta\rho}{}^{21})\,d\xi,$$

$$L_{\delta\rho}{}^{12}(\xi) = L_{\delta\rho}^{(0)12} - \frac{1}{2}\int_0^\xi \gamma_3 d\xi\,(L_{\nu\nu}{}^{21}\delta_{\rho\delta} - L_{\delta\rho}{}^{21}) - \frac{1}{2}\int_0^\xi (\gamma_1 L_{\nu\nu}{}^{12}\delta_{\rho\delta} - \gamma_2 L_{\delta\rho}{}^{12})\,d\xi.$$

In order to compute the loop shown in Fig. 2b, we must evaluate the integral

$$\int_0^\xi (L_{\delta\rho}{}^{12}(\eta)L_{\rho\delta}^{*21}(\eta) + L_{\delta\rho}{}^{21}(\eta)L_{\rho\delta}^{*12}(\eta))\,d\eta.$$

For the elastic moduli, $L_{\delta\rho}^{(0)12} = L_{\delta\rho}^{(0)21} = \delta_{\rho\delta}$, and we obtain

$$L = \exp\left\{-\int_0^\xi \left(\frac{1}{2}\gamma_3 + \frac{1}{4}\gamma_4 + \frac{3}{4}\gamma_1\right)d\eta\right\}.$$

Thus, when the electron-electron interactions are taken into account the expressions (8) acquire the extra factor $\Phi(\ln T) > 0$, where

$$\Phi(\xi) = \int_0^\xi L^2(\eta)\,d\eta. \tag{16}$$

The signs of the corrections and the relation $\frac{1}{2}\delta C_{11} = -\delta C_{12}$ remain unchanged.

Thus, we can state that in a reasonably good sample the structural transition always precedes the transition to the superconducting state. If the electronic interaction constant is small, then the terms studied in Sec. 2 are themselves capable of making the elastic modulus $C_{11} - C_{12}$ vanish. If, however, the vertex part becomes infinite at some temperature T*, then, according to (16), the vanishing of the modulus $C_{11} - C_{12}$ occurs at temperatures close to, but higher than, T*. In fact, near the pole [11]

$$\Phi \propto \left(1 + g_1 \ln\frac{\tilde{\omega}}{T}\right)^{-1/2}.$$

This result is very important for the understanding of the connection between the high-temperature superconductivity and the instability in the β-W structures.

It was noted above that the optical frequencies also soften.[6)] Since, for example, the "sublattice" displacement in a chain transforms according to the same representation as $\epsilon_{xx}-\epsilon_{yy}$, the vibrational energy includes terms of the type (7) containing combinations of u_z^2 and $u_z(\epsilon_{xx}-\epsilon_{yy})$. Therefore, when the three-dimensionality of the phonons is taken into account, the question as to which frequencies—optical or acoustic—vanish first depends on the magnitudes of the deformation potentials and on the relation between the elastic moduli and the optical frequencies at high temperatures. In compounds of the type Nb_3Sn or V_3Si, this question is experimentally resolved in favor of the acoustic vibrations. Because of the cross terms $(\epsilon_{xx}-\epsilon_{yy})u_z$, the sublattice displacement, generally speaking, develops simultaneously with the tetragonal deformation [12].

Let us now touch upon the question of the effect of stresses and impurities, or structural defects, on the transition. According to Table II, the strains for an individual chain have both "diagonal" and "nondiagonal" representations. As for the former, their role consists in changing the chemical potential, i.e., in the doping of the d bands with s-band electrons. It is not difficult to verify that the matrix elements for the Cooper-type diagrams do not change, whereas in the "zero-sound" channel of the vertex part, i.e., in (8) or (16), the logarithmic integrals are cut off at the strain-energy value, as a result of which the structural transition is suppressed at a sufficiently large value of the energy.

As to the vertex part itself, it depends on two logarithmic parameters:

$$\eta=\ln\frac{\tilde{\omega}}{A\varepsilon_{ii}},\qquad \xi=\ln\frac{\tilde{\omega}}{T}$$

and was found earlier in [10]. The spinor combination $\gamma_1+\gamma_2$, responsible for the Cooper pairing, is γ_3 in the notation of [10] $(\eta<\xi)$:

$$\gamma_3(\xi,\eta)=\frac{g_1}{(1+g_1\eta)^{1/4}(1+g_1\xi)^{3/4}}\exp\left\{-\frac{g_1}{2}(\xi-\eta)\right\}. \qquad (17)$$

It was shown in [10] that the equation for the superconducting gap coincides with the homogeneous parquet equation for the function γ_3 and has a solution if the latter has a pole. If the magnitude of the strain is such that $A\epsilon_{ii}$ is higher than the cutoff energy $\tilde{\omega}$, then the parquet equation degenerates into the standard ladder of the Cooper diagrams of the BCS theory.7)

Let the strain belong to the "nondiagonal" representation of $\epsilon_{xx}-\epsilon_{yy}$. In this case the spectrum of the electrons of a chain becomes dielectric, and all the logarithmic integrations are cut off at energies of the order of $D_1(\epsilon_{xx}-\epsilon_{yy})$. Thus, an arbitrary large strain, generally speaking, destroys both the structural instability and the Cooper pairing.

Let us discuss on the basis of this qualitative picture the experimental data on the nature and magnitude of the anharmonic effects. Such data (see the references in [1]) are for the present not many, and they pertain primarily to the vicinity of the transition temperature. From the general standpoint the appearance of strong anharmonicities and the dependence of all the parameters on the strain are well understood from the foregoing. The parquet approximation, however, cannot describe the phase transition itself, especially since a second-order phase transition cannot in general be realized in the purely one-dimensional model, and the question remains: How does the interchain interaction make such a transition possible? Let us note at once in this connection that from the point of view of the full cubic group, a purely tetragonal strain [19], or a deformation accompanied by a displacement of the transition-element atoms in the chain, a displacement which has been observed in Nb_3Sn [12], can be realized only through a first-order phase transition. The so-called martensitic transition is probably a second-order transition. For a single chain, a second-order phase transition is not forbidden. In fact, after the imposition on the chain of tetragonal strain and the displacement of the sublattices, the remaining point group has half the initial number of symmetry elements and possesses only one-dimensional representations. Therefore, in the Landau expansion of the theory of second-order phase transitions, there are no third-order terms for the individual chains: they arise only as a result of a weak interaction between the chains.

From the condition $D_1(\epsilon_{xx}-\epsilon_{yy})\sim T_m$, we obtain the correct order of magnitude for the strain: $\epsilon\sim u_z\sim T_m/D_1\sim 10^{-3}$. For $T>T_m$ the values of the strain at which the anharmonic effects are important are determined by the estimate

$$\varepsilon,\ u_z\sim 10^{-3}T/T_m. \qquad (18)$$

The data on the dependence of T_c and the elastic moduli on uniaxial strain ($\epsilon_{yy}=\epsilon_{zz}$, ϵ_{xx}) easily fit into the expounded scheme. Indeed, the logarithmic contribution to the elastic free energy (5) from the two systems of chains (along the [010] and [001] directions) is cut off at $D_1\epsilon$, which implies an increase in the stiffness of the lattice in comparison with the case when there is no strain (it is assumed that $T<D_1\epsilon$). The order of the change in the elastic moduli, $\Delta C/C\sim 1$ for $\epsilon\sim 10^{-3}$ T/T_m, turns out to be correct [1]. The superconducting transition should then be attributed to the family of chains along the [100] direction. The latter circumstance apparently allows a direct experimental verification in, for example, the measurements of the conductivity anisotropy function in the presence of strain. No quantitative data exist on the logarithmic dependence at high temperatures of the elastic moduli on strain in the region (18). At low temperatures, this dependence, like (9) and (9′), is quadratic [1].

Hydrostatic pressure leads to a homogeneous compression. As was indicated above, this effect would consist in the redistribution of the electrons between the s and d bands, and, in the parquet approximation, the superconducting transition point would, according to (17), not be affected. If we assume that the entire pressure dependence of the elastic moduli is connected with the contribution (7) from the d electrons, then the expressions (8) should be replaced by the following ones:

$$\delta C_{11}=-\frac{2D_1^2}{a^2\pi v}\left\{\ln\frac{\tilde{\omega}}{T}+\varphi\left(\frac{A\varepsilon_{ii}}{T}\right)\right\},\qquad \delta C_{12}=-\frac{1}{2}\delta C_{11}; \qquad (19)$$

$$\varphi(z)=\int\limits_{-\infty}^{+\infty}\frac{dx}{4x}\left\{\operatorname{th}\left(x+\frac{z}{2}\right)+\operatorname{th}\left(x-\frac{z}{2}\right)-2\operatorname{th}x\right\}. \qquad (20)$$

According to (8) and (20), C_{11} and $C_S=\frac{1}{2}(C_{11}-C_{12})$ increase, while C_{12} decreases, with increasing pressure. Further, if the temperature-dependent term in C_{44}, which is usually less than δC_{11}, is also due to a contribution of the type of Fig. 6a, then, as we shall show below, it is proportional to δC_{11}, differing from it in the magnitude of the coefficient in front of the logarithm. Therefore, C_{44} also increases when $\epsilon_{ii}\neq 0$. Further-

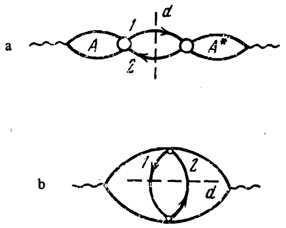

FIG. 6

more, from (19) follows the assertion that in the high-temperature region the pressure derivatives $\partial C/\partial P$ relate to each other in the same way as their temperature-dependent terms, i.e.,

$$\frac{C_{ij}'}{C_{lm}'}=\frac{C_{ij}(T_1)-C_{ij}(T_2)}{C_{lm}(T_1)-C_{lm}(T_2)}. \qquad (21)$$

Experiments on the effect of pressure have been performed by Carcia et al.[20] for V_3Si and V_3Ge right up to pressures of 10 kbars. Their result for V_3Si is that C_{44} and C_{11} increase, while $C_S = \frac{1}{2}(C_{11}-C_{12})$ decreases, with increasing pressure.

It is significant, however, that all the derivatives have the same order of magnitude, $\partial C/\partial P \sim 1$, as those for normal metals. Meanwhile, at these pressures $\epsilon_{ii} \sim 10^{-3}$, and, according to (19), large anharmonic effects might have been expected. Notice, incidentally, that the elastic moduli in the formulas (19) would then vary at low pressures according to a quadratic law. The fact that hydrostatic compression does not reveal strong anharmonicities indicates, in our opinion, that the d and s bands are not in communication.

There arise in the structural transition strains which make the electron spectrum in the two chain systems dielectric. (As far as we know, no measurements have been made of the anisotropy in the conductivity.) It is also known how T_c and T_m get separated in the nonparquet approximation. They are, however, of the same magnitude, and therefore a change in T_m by a value of the same order as itself implies (for a pure sample!) the same change in T_c, although the relative sign of the effect is theoretically unknown. The application of pressure changes the elastic moduli by values typical for all solids. Therefore, the quantity $\partial T_c/\partial P = 0.036$ K/kbar found by Smith [21] for V_3Si seems to be correct and agrees with the data obtained by Carcia et al.[20]:

$$\frac{1}{T_m}\frac{\partial T_m}{\partial P} \sim \frac{1}{C}\frac{\partial C}{\partial P},$$

if we assume that the pressure P^* that changes the lattice constant significantly is equal to $P^* \sim 10^6$ bar.

Uniaxial strains, as has already been indicated, strongly influence the electron spectrum and, consequently, T_m. We obtain the estimate for the quadratic effect of the variation of T_m at not too large values of the tetragonal strains in the same manner as we derived the expression (20):

$$\frac{\Delta T_m}{T_m} \propto \frac{|\Delta T_c|}{T_c} \sim -\frac{D_1{}^2\varepsilon^2}{4T_m{}^2} \sim -10^5\varepsilon^2.$$

The estimate obtained by Testardi [1] gives $\Delta T_c/T_c \sim -10^4\epsilon^2$.

The role of impurities and defects is less well understood, since in a one-dimensional chain the defects, generally speaking, localize the conduction electrons. If, however, the impurity atom is a sufficiently close neighbor of the nontransition-element atom in the periodic table, as, for example, Al and P for Si, or In and Sb for Sn, then it may be inferred that at low concentrations their role is primarily one of doping the compound, i.e., of shifting the chemical potential. As was noted above, such an effect should enhance the stability of the system. The effect of doping has been studied for the systems $Nb_3Sn_{1-x}Sb_x$ and $Nb_3Sn_{1-x}Al_x$ (see [1]). The structural-transition point is clearly depressed at low concentrations. Recomputing the concentration x for the equivalent change in the chemical potential, we find that a change in T_m of the order of unity occurs at

$$x \sim \frac{\nu_d}{\nu_s}\frac{T_m}{E_F} \sim \frac{\nu_d}{\nu_s}\cdot 10^{-3},$$

where ν_d and ν_s are the densities of states for the d and s bands respectively. For the $Nb_3Sn_{1-x}Al_x$ systems the limit of existence of the tetragonal phase is indicated in [22]: $x < 0.07$. Taking into account the ambiguity about such experiments in connection with the ambiguity about the preparation of even pure samples, we should consider the agreement to be a good one if $\nu_d/\nu_s \sim 10$. In this connection, we should like to point out that the role of impurities in any case does not amount to changing only the lattice constant, i.e., it is not comparable to the action of pressure, although we can, in relation to the dependence of the elastic moduli on doping, repeat everything that has been said apropos of (19).

Let us now turn to the question of the temperature dependence of the modulus C_{44}. Figure 6a shows the contribution to C_{44} that arises as a result of the electron interaction. The wavy line corresponds to the off-diagonal component of the strain tensor. The portions of the diagram denoted by A and A* can be of twofold character. First, they could be nondiagonal transitions for the states in the d band, transitions which are connected with the fact that the interaction (14) has a component corresponding to the requisite representation. For example, according to the Table II, this will be $B_2^-(\sigma_z p_z \epsilon_{xy})$ for the functions X_2 and X_4, and $B_1^-(\epsilon_{xy}p_z)$ for the functions X_1 and X_3. The expressions for A and A* do not themselves contain logarithmic contributions, since because of the additional p_z, the integration domain lies far from the Fermi point at X. The internal cross section yields a contribution to C_{44} of the form

$$\delta C_{44} = -\frac{|A|^2}{2\pi\nu a^2}\ln\frac{\tilde{\omega}}{T}. \qquad (22)$$

Notice that the contribution of the diagram of Fig. 6b is unimportant, since the logarithmic singularity of the parquet insert is integrated over the variables in A and A*. If a set of functions of the type X_2 and X_4 are realized at the point X, then besides the assumed weakness of the interaction, $|A|^2$ contains in addition the square of the spin-orbit interaction constant. In the case of the representations X_1 and X_3, the choice of $B_1^-(\epsilon_{xy}p_z)$ implies only the assumption of the smallness of the interaction constants in the parquet equations. In this case the order of magnitude of this contribution to C_{44} could be regarded as reasonable.

Let us consider the other possibility when the portions A and A* of Fig. 6a pertain to s electrons. The diagram of Fig. 6b is again unimportant. As to the interaction vertex γ^{sdsd} corresponding to the scattering of s electrons by d electrons, there are no grounds for supposing that it is very small. Notice that it is precisely this interaction that participates in the production of the self-consistent field for the individual chains. Thus, this mechanism also leads to the expression (22).[8]

Finally, if γ^{sdsd} has an exchange part, then we obtain for the correction to the susceptibility a paramagnetic contribution that increases with decreasing temperature. A weak point of this susceptibility-growth mechanism is that the weakness connected with the exchange interaction figures in it. According to Fig. 3, the change $\Delta\chi/\chi$ for the 300–100-K range is roughly 30% in V_3Si, whereas for C_{44} this change is about 4%[1]. Of course, the latter circumstance can easily be related to the numerical smallness of the components of the deformation potential, since the distribution of the s electrons is near-isotropic. In fact, the Young modulus for V_3Si is observed to be isotropic at high temperatures. This is not so in Nb_3Sn, and the corresponding change in C_{44} is also markedly larger.

4. CONCLUDING REMARKS

The contents of the preceding two sections demonstrate, to our mind, that the expressed ideas about the predominant role of the linear chains consistently describe the numerous peculiar properties of the high-temperature superconductors with the A-15 structure. At high temperatures, this description is of quantitative nature. The elastic properties are completely adequately accounted for by the theory. For the magnetic susceptibility and the Knight shift the presence of temperature-dependent terms of both signs and diverse natures allows us to understand why, generally speaking, the magnetic properties quite significantly vary from compound to compound.

From the proposed standpoint, the importance of further experimental study of these compounds lies in the fact that, first, the experimental situation indicates the existence in nature of one-dimensional structures with a sufficiently weak interchain interaction, and, secondly, it positively answers the theoretically unclear question of the possibility of the earlier investigated [10,11] phase transitions in quasi-unidimensional chains if the latter are placed in a three-dimensional medium.

If the structural transition is, as was discussed in Sec. 3, due to the electron interactions, then the superconducting transition temperature T_c should be expected to differ from T_m by only a small factor. The question of the role of the anharmonicities in the elevation of T_c reduces to the question as to whether the dielectric splitting of the electron spectrum has time to develop to such an extent that the electronic vertex part may no longer become infinite. It was shown above that, in principle, impurities and the effect of doping are capable of decreasing the magnitudes of the dielectric splitting, thereby raising T_c.

Thus, in a system possessing a well-defined one-dimensional structure, and about which it is known that either its symmetry permits the degeneracy of the electronic levels with $\partial\epsilon/\partial p \neq 0$, or the electrons do not fill the entire one-dimensional band, the detection of a structural instability is an indication of the possibility of a superconducting transition at a nearby temperature.

Let us explain further the difference in the relation between superconductivity and structural instability in the three-dimensional and one-dimensional cases. In the first case there is practically no connection between them. According to the BCS theory, the larger the effective interaction constant, the higher T_c. The former is determined on the average by the interaction with the various phonon modes and the Coulomb interaction. The numerical computations of [23], however, show that if this constant is sufficiently large, then the structure is unstable. In contrast to the exponential BCS formula, the transition temperature of the corresponding phase transformation is determined by the anharmonic interactions and is therefore, generally speaking, high compared to T_c. Therefore, after the structural transition, we again have to deal with a BCS constant that does not exceed the permissible stability limit, from which the maximum possible value of T_c can be estimated. In the region very close to, for example, a shear-type structural transformation temperature, the frequency of the selected vibration branch tends to zero, but as has been noted, the effective interaction constant determining T_c if averaged over the entire phonon spectrum. Because of this, no significant enhancement of the interaction occurs even in the vicinity of the structural transition.

In the one-dimensional case, a large interaction constant also implies an instability of the system. The difference, however, is that any attempt to decrease the energy of the system through deformation leads to the appearance of a dielectric gap in the spectrum, and this competes with the possibility of achieving Cooper pairing through the same means. This is a peculiar property of an electron spectrum that coincides with the hole spectrum; in metals, a small deformation does not qualitatively change the spectrum near the Fermi surface. Thus, in this conception, instability and superconductivity are two aspects of one and the same phenomenon: the instability of the electron spectrum against interactions involving attraction.

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[1] The possibility of an antiferromagnetic ordering has also been demonstrated by Dzyaloshinskiĭ and Larkin [11].

[2] Here and below all the quasi-momenta are reckoned from the point $X\{0, 0, \pi/a\}$.

[3] The contribution from the simple loop in Fig. 2 contains, generally speaking, a power-law dependence on T, of smallness T^2/E_p^2. We neglect such small terms.

[4] This interaction should be thought of as due both to direct d-electron transitions between the orthogonal chains and to exchanges via the s electrons.

[5] Here our results differ from those of [11].

[6] In the present case only those modes which transform according to the requisite representations in Table II can be involved. The rest are, in general, not linked to electrons in the basic approximation.

[7] No change occurs in the integrals in the "zero-sound" channel when the crystal is doped if we consider a transition with the formation of a superlattice. The author is grateful to I. E. Dzyaloshinskiĭ for this remark. However, the nature of the transition cannot be elucidated in our approximation.

[8] In other words, an interaction that leaves the spectrum plane can lead in the representation B_2^- of Table II to large terms that are proportional to the field or the strains.

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173