approximately over 10 realizations of f. The absolute error in the calculation of the mean value did not exceed 0.01. As $r_0 \to 0$, the values of the potentials at the points turn out to be entirely uncorrelated, and we obtain the results of the lattice problem of nodes, $\nu_c = 0.32$ [7]. At $r_0 \gg 1$, ν_c ceases to depend on r_0, corresponding to the transition to the continual problem. The limiting value of ν_c is indeed the critical fraction of the volume, which is of interest to us. We obtained similar results for the other potentials mentioned above.

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ROLE OF LINEAR CHAINS IN THE FORMATION OF THE PROPERTIES OF SUPERCONDUCTORS WITH A-15 STRUCTURE

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It is shown that the elastic properties of superconductors with β-W structure follow from the assumption that the α-electron energy spectrum is almost flat.

Superconductors of the A_3B type have a interesting property in that the transition to the superconducting state is a structural transition at a temperature T_m close to T_c, and if there is no transition obtained, a tendency to this transition is observed, manifest in a softening of the corresponding elastic moduli [1, 2]. In all the known cases, T_m differs from T_c by not more than a factor of two, whereas the temperature dependences that anticipate the transition extend to temperatures 300 - 400°K.

It was noted in [3] that owing to the small overlap of the shells, an important role in the structure of β-W can be played by three systems of linear chains of transition-element atoms. The approximation of strong coupling of the d-electrons in the chain was involved to one degree or another in all the subsequent studies [4 - 6], in which an anomalously large density of states $\nu(\varepsilon_F)$ was assumed, owing to the singular behavior $\nu(\varepsilon) \sim \varepsilon^{-1/2}$ at the edge of the one-dimensional band.

It is shown below that the main properties of this group of compounds can be understood within the framework of the concrete symmetry of the A-15 structure on the basis of the concepts of the Fermi-liquid theory, with allowance for the changes introduced by the one-dimensional character of the filaments. Indeed, in a one-dimensional metal the Cooper pairing is connected with the Peierls doubling of the period [7]. It will be made clear below that it is also connected with the tetragonal deformation in the β-W structure. The literature contains discussions both of the non-phonon superconductivity mechanisms in these compounds and of the role of the structure instability in the increase of

T_c. In our opinion, there are still no grounds for the first question. The proposed answer to the second question is that in A-15 the proximity of the superconducting and structural transitions is the consequence of the almost flat spectrum of the d-electrons. The relatively large values of T_c and T_m ($\sim$20°K) are apparently the result of the larger state density, in the mean, in the narrow d-band, a measure of which is the value of the electronic specific heat.

The circumstance that suggests the concepts of [7] is the logarithmic dependence [2] of the elastic moduli, $C_{ij} = a + b \ln T$. In the substance most thoroughly investigated, V_3Si, the dependence is most strongly pronounced for C_{11} and C_{12}, and the change of C_{44} is relatively small. In Nb_3Sn the difference between C_{11}, C_{12}, and C_{44} is smaller.

According to [7], the metallic states of a one-dimensional chain exhibit instability in the presence of attraction simultaneously with respect to superconducting pairing and doubling of the period[1]). The doubling of the period in an individual chain of Nb atoms was indeed observed [9] in a structural transition in Nb_3Sn. However, for each period of the β-W lattice there are two atoms of the transition metal in the chain, so that the logarithmic corrections to the phonon frequencies of [7] pertain to a phonon momentum q = 0.

In the one-dimensional case, unlike in the BCS theory, it is impossible to obtain formulas in closed form for the description of the transition, even in the weak interaction limit. It can be seen [7, 8], however, that

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

where $\bar{\omega}$ is an energy on the order of the Debye temperature, and g is the effective dimensionless constant of the interelectronic interactions. We have [2]

°K	Θ_D	T_m	T_c
V_3Si	~500	18 - 25	17
Nb_3Sn	~300	~43	18.2

Therefore g is not too small. For V_3Si the situation is apparently more favorable. We confine ourselves henceforth to structural properties at high temperatures.

If $D\varepsilon\psi^+\psi$ is the Hamiltonian of the interaction of the electrons with the deformation ε, then the increment quadratic in ε to the density of the free energy is

$$\frac{\epsilon^2}{2} D^{\alpha\alpha'} D^{\beta\beta'} \left[\int G_p^{\alpha} G_p^{\alpha'} \delta_{\alpha'\beta'} \delta_{\alpha\beta} d^2p + \iint G_p^{\alpha} G_p^{\alpha'} \mathcal{T}_{\lambda\mu}^{\alpha\beta\alpha'\beta'} G_p^{\beta} G_p^{\beta'} d^2p d^2p' \right]. \tag{2}$$

Here $\int d^2p = (2\pi)^{-1} T \sum_{\omega} \int dp$, G_p is the Green's function, α is the index of the band and $\mathcal{T}$ is the electronic vertex part. Near the Fermi surface we have $G_p^{\alpha} = a(i\omega - \varepsilon_p^{\alpha})^{-1}$.

In the A-15 lattice, as already noted, there are two atoms per period for each chain. Therefore the electron spectrum of an individual filament in the crystal field splits into bands, and each band, if we disregard the flow from the s-band to the d-band, is generally speaking either completely empty or

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[1])The possibility of antiferromagnetic ordering was also demonstrated in [8].

completely filled. In the space group O_h^3, however, the spectrum at the points X, owing to the presence of nontrivial translations, is always doubly degenerate without allowance for the spin [10]. The filling of the one-dimensional Brillouin zone can therefore be compatible with the metallic properties of the chain electrons. The behavior of the terms near the point X can be easily obtained by the usual methods (see [11]). The wave-vector group at the point X is isomorphic to the corresponding diamond-lattice group, and differs from it in the orientations of nontrivial elements relative to the principal axes. Without allowance for the spin, there are four representations $\{X_1, X_2, X_3, X_4\}$ (the notation is that of [11]). The Hamiltonian for the representations $\{X_2, X_4\}$ is

$$\hat{H} = A_1 p_x^2 + B(\epsilon_{yy} + \epsilon_{zz}) + v\hat{\sigma}_z p_x + \hat{\sigma}_x[D_1(\epsilon_{yy} - \epsilon_{zz}) + D_2 u], \tag{3}$$

where u is the displacement of the "sublattices" along the filament. It follows from (3) that the deformation $\varepsilon_{yy} - \varepsilon_{zz}$ gives rise to transitions between bands, with energy $\pm vp_x$. As to the representations $\{X_1, X_3\}$, for an individual filament (neglecting the dependence on p_y and p_z) the spectrum corresponds to double degeneracy at all p. The completely filled band does not conduct in this case, and a half-filled band would correspond to other singularities, for example, the doubling of the period of the A-15 lattice.

According to (3), the contribution made to the first term of (2) from the system of filaments along (100) (per unit volume) is

$$\delta F_x = -\frac{D_1^2}{2\pi v a^2}(\epsilon_{yy} - \epsilon_{zz})^2 \ln\frac{E_F}{T}, \tag{4}$$

where E_F is the cutoff energy ($\sim$1 eV) and a is the lattice period. Summing over all the orthogonal filaments, we get

$$\delta C_{11} = -\frac{2D_1^2}{a^2\pi v}\ln\frac{E_F}{T}; \quad \delta C_{12} = \frac{D_1^2}{a^2\pi v}\ln\frac{E_F}{T}. \tag{5}$$

Allowance for the second term in (2) leads to a multiplication of each of the expressions (5) by a factor in which the first terms (with logarithmic accuracy [7]) are given by

$$\Pi \approx \left\{1 - g\ln\frac{E_F}{T}\right\}, \tag{5'}$$

where g is the effective interaction between the electron and includes the interaction via the optical phonons[2)]. Thus, deviations from a linear logarithmic dependence occurs when $g\ln(E_F/T) \sim 1$. At $g < 0$, an infinite value of $\mathcal{T}$ would correspond to a pure electronic transition at the temperatures (1). It is important that the vanishing of the elastic modulus $C_{11} - C_{12}$ occurs earlier, since the singular part [8] in Π is proportional to $[1 + g\ln(E_F/T)]^{-1/2} > 0$. Thus, in a pure sample a tetragonal deformation anticipates a superconducting transition. The frequencies of the optical phonons decreases logarithmically, but at $C_{11} - C_{12} = 0$, in accord with experiment, they remain finite. Their vanishing would coincide with $\mathcal{T}$ becoming infinite.

[2)] Acoustic phonons make no contribution to the electron interactions in the one-dimensional case.

So far, C_{44} was independent of the temperature. The terms that lead to logarithmic additions to C_{44} are due to the coupling between the s and d electrons: $\gamma^{sd}G^{1d}G^{2d}\gamma^{ds}$. The contribution from these terms is proportional to the square of γ^{sd} and, although there are no particular reasons for γ^{sd} being small, this can explain the relatively weaker dependence of C_{44} on lnT. For example [2], for Nb_3Sn the absolute change of C_{11} in the interval from 300 to 100°K is five times larger than the change of C_{44}. According to (5), the slope of the plot of C_{11} against lnT should be twice as large as for C_{12}. It is still too early to speak of a quantitative agreement with the mentioned fact, which is a consequence of the symmetry, although the picture is qualitatively correct [2].

Most data on the elastic moduli were obtained from measurements of the speed of sound. Static measurements of elastic moduli are subject to large spreads and agree poorly with ultrasonic measurements. We note in this connection that the picture described above leads to an important new circumstance - the dispersion of the elastic moduli at wave vectors $qv \gtrsim T$. For example, longitudinal sound propagating along (100) corresponds to a modulus C_{11}, which is given at $qv \gg 4\pi T$ by

$$\delta C_{11}(q) = -\frac{2D_1^2}{a^2\pi v}\left\{\ln\frac{E_F}{T} - \frac{1}{2}\ln\frac{vq}{4\pi T}\right\}. \qquad (6)$$

Neutron measurements of the phonon spectrum (see [2]), while pointing to the existence of such an effect, are not sufficient for a comparison of (5') and (6).

A structural transition with tetragonal deformation and sublattice displacement [9] should be of a first-order transition for the cubic group. Experiment, as is well known, favors a second-order transition. The values of the deformations also indicate the same: $\varepsilon \sim u \sim T_m/E_F \sim 10^{-3}$. The contradiction is eliminated by the fact that a second-order phase transition is possible for an individual filament. Indeed, according to (3), $\varepsilon_{yy} - \varepsilon_{zz}$ and u belong to the same representation. The symmetry group of the new phase has only one-dimensional representations. The weakness of the first-order phase transition is due by the same token to the smallness of the interaction between the filaments. If the latter is denoted by $V_{12} \equiv \mathcal{J}^{sdss}$, then the deviations of the d-electron Fermi surfaces from planes will be characterized by energies V_{12}^2/E_F, which should be small in comparison with the temperature. The estimate of V_{12} therefore takes the form

$$V_{12} < \sqrt{T_m E_F} \sim 10^{-1} - 10^{-2}\ \text{eV}.$$

This seems not too unlikely, if one recognizes the weakening of the exchange between the filaments as a result of their packing in the lattice of the nontransition atoms.

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INSTABILITY OF METALLIC HYDROGEN STRUCTURE TO SMALL CHANGES IN THE ALLOWANCE FOR THE ELECTRON-ELECTRON INTERACTION

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The binding energy of metallic hydrogen at zero pressure is calculated numerically in second and third order perturbation theory. It is shown that small changes in the allowance for the electron-electron interaction can lead to the vanishing of the metastable "metallic" minimum of the total energy.

The question of the existence of metastable metallic hydrogen is of considerable interest and is discussed in a number of papers [1 - 3].

The most fundamental calculations of the possible metastable structure at zero pressure were performed in [2] and led to the unexpected conclusion that there exists a metastable filamentary structure in which the protons lie close together along parallel filaments, which intersect a perpendicular plane in a lattice made up of regular triangles.

The binding energy was calculated in [2] with inclusion of second and third order perturbation-theory terms in the electron-proton interactions. A number of approximations were made, due to the inaccuracy in the allowance for the interaction of the electrons with one another. In the second-order term, this reduces to an inaccuracy of the employed formula for the dielectric constant of a homogeneous electron gas. In the third-order terms there are also correlation corrections, which have not been taken into account at all in [2].

The second source of errors is the discarding of the higher orders of perturbation theory. In fact, however, it is impossible to calculate the fourth-order terms with present-day computers.

The purpose of the present paper is to ascertain the influence of small corrections, connected with allowance for electron-electron correlations in second and third order of perturbation theory on the qualitative statements made concerning the character of the metastable structure of metallic hydrogen.

The simplest diagrams that take into account the correlation corrections to the energy of the ground state of an electron gas in the external field of the lattice protons are shown in Fig. 1a for the second-order term and in Fig. 1d for the third-order terms. The corresponding integrals can be obtained only numerically. The most widely used method of taking such diagrams into account is to replace in the first diagram the Coulomb potential, which corresponds to the internal wavy line, by a certain effective mean value $V_{eff} = V_c(k^2 + p_F^2)^{1/2}$, where p_F is the Fermi

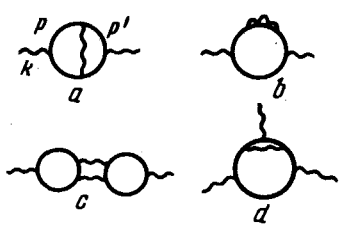

Fig. 1