

# Singularities of the electronic spectrum of compounds with $\beta$ -W structure

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It is shown that the overlap of filaments of transition elements leads to singularities in the electronic density of states, and these singularities account for the anomalous properties of these compounds.

In the universally accepted theory<sup>[1]</sup> of the properties of compounds such as  $\text{Nb}_3\text{Sn}$  and  $\text{V}_3\text{Si}$ , the Fermi level is assumed to be close to the bottom of one of the empty  $d$  bands with large (one-dimensional) density of states. This choice is accidental. The author has noted<sup>[2]</sup> that if the electron bands do not cross, then from the point of view of the occupational numbers the Fermi level must pass through the point  $X$ . The singularities of the spatial symmetry then ensures a large Fermi surface; the absence of the usual  $T^5$  dependences from the temperature dependence of the resistance (see<sup>[3]</sup> and<sup>[4]</sup>) is strong evidence that  $s$ -electrons do not take part in the conductivity of these compounds.

The theory<sup>[1]</sup> leads to temperature increments to the elastic moduli, in the form

$$C_{ij} = A + B \ln T. \quad (1)$$

What is surprising, however, is that slow variations with temperature are observed in experiment all the way to  $T \sim T_m \lesssim 100^\circ\text{K}$ , when the interacting-filament approximation can hardly be valid. In addition, although the experimental data on the susceptibility<sup>[5]</sup> of  $\text{V}_3\text{Si}$  are plotted in the form (1), it is difficult to understand, in light of the selection rules,<sup>[1]</sup> the large change of the susceptibility.

A general expression for the energy spectrum of the electrons in the vicinity of the point  $X$  is<sup>[11]</sup>

$$\epsilon_{1,2} = c(p_x^2 + p_y^2) \pm \{v^2 p_x^2 + c'^2(p_x^2 - p_y^2)\}^{1/2}. \quad (2)$$

Here  $c$  and  $c'$  are small to the extent that the interaction between the filaments is small. The order of magnitude  $c/a^2 \approx T^*$  ( $a$  is the lattice constant) characterizes temperatures to which formulas<sup>[11]</sup> are valid. We see, however, that (2) implies a fine structure of the state density, with a scale  $T^*$  ( $dp_x/d\epsilon$  and the areas of the Fermi surface near the boundary of the Brillouin zone depend on  $\epsilon$ ). Confining ourselves to transitions between the nearest filaments, we obtain the energy spectrum at the boundary of the zone:

$$\tilde{\epsilon}_{1,2} = \sin^2 \phi + \sin^2 \psi \pm \{ \pi_x^2 + (\sin^2 \phi - \sin^2 \psi)^2 \}^{1/2}. \quad (2')$$

where we have introduced the dimensionless variables

$$\epsilon = 2(v/a)\lambda\tilde{\epsilon}; \quad (2\phi, 2\psi) = (p_x a, p_y a); \quad \pi_x = 2p_x \lambda a, \quad (3)$$

and the quantity

$$\lambda = 2(Ba/v)^2 \quad (3')$$

contains the square of the ratio of the "exchange integral"  $B$  to the width of the zone. Thus, the scale of  $T^*$  is  $\sim 10^2$  °K (see below). From the dispersion law (2') we can easily obtain an expression for the density of states in terms of elliptic integrals. Thus, at  $\tilde{\epsilon} < 0$  we have

$$\nu(\epsilon) / \nu(0) = (4/\pi^2) E(k)K(k); \quad k^2 = 2/2 - \tilde{\epsilon}. \quad (4)$$

Here  $\nu(0)$  is the volume density of states for a flat spectrum. For one face of the cube and for one spin we have

$$\nu(0) = 1/2 \pi v a^2. \quad (5)$$

At  $x = \tilde{\epsilon} \rightarrow 0$  and  $x = \tilde{\epsilon} - 2 \rightarrow 0$ , Eq. (4) has a logarithmic singularity

$$\nu(\epsilon) = \nu(0) \frac{2}{\pi^2} \ln \frac{32}{|x|}. \quad (4')$$

It can be shown that  $\nu(\epsilon)$  is symmetrical with respect to the substitution  $\tilde{\epsilon} \rightarrow 2 - \tilde{\epsilon}$ . Therefore a stoichiometric composition corresponds to the choice of the chemical potential at the point  $\tilde{\mu} = 1$ . Since  $T^* \sim 10^2$  eV, doping by 1% or a fraction of a percent shifts the Fermi level appreciably. We assume that samples that undergo a structure transition correspond to the Fermi level  $\tilde{\mu}$  near the singularity (4') ( $\tilde{\mu} \rightarrow 0$ , as  $\tilde{\mu} \rightarrow 2$ ).

We present the results. For the temperature-dependent increment to the paramagnetic susceptibility we obtain ( $T < T^*$ ):

$$\chi(T) = \chi_0 \frac{2}{\pi^2} \ln \frac{64 \gamma T^*}{T} \quad (6)$$

For the electronic component of the specific heat  $c_e$  we have

$$c_e(T) = c_{e0}(T) \frac{2}{\pi^2} \ln \frac{16 T^*}{T} \quad (7)$$

$c_{e0}$  and  $\chi_0$  are the electronic specific heat and the paramagnetic susceptibility in the case of a planar dispersion law ( $c$  and  $c' = 0$  in (2)).

Similar logarithmic relations result from the electronic contribution to the elastic moduli. For a filament along the  $z$  axis, the electron spectrum depends on the strains:

$$\tilde{\epsilon}_{1,2} = \sin^2 \phi + \sin^2 \psi + d_2 \epsilon_{zz} \pm \{ \pi_x^2 + (\sin^2 \phi - \sin^2 \psi + d_1(\epsilon_{xx} - \epsilon_{yy}))^2 \}^{1/2},$$

where  $d_1$  and  $d_2$  are the components of the deformation potential. We present an expression for the contribution made to the elastic energy by one filament, normalized to separate the logarithmic term  $\ln(\tilde{\omega}/T^*)$ , from the energy region  $\tilde{\omega} \gg \epsilon \gg T^*$  (cf. [11]).

$$\left( \ln \frac{\tilde{\omega}}{T^*} + \text{const} + \frac{2}{\pi^2} \ln \frac{32 T^*}{T} \right) (\epsilon_{xx} - \epsilon_{yy})^2 + \frac{2d_2^2}{\pi^2 d_1^2} \ln \frac{32 T^*}{T} \epsilon_{zz}^2 \quad (8)$$

The values  $q^* v = 2\pi T^*$  determine the characteristic scale of the phonon dispersion  $\omega(q)$ . Determining  $a/v = 2\pi N(0)/3$  from (5), we obtain in  $\text{Nb}_3\text{Sn}$   $\xi^* = aq^*/\pi \sim 0.1 - 0.2$ , in accordance with the results of [61].

Finally, the singularity in the Cooper channel acquires a doubly-logarithmic character

$$g_1 \ln \frac{\tilde{\omega}}{T} \Rightarrow g_1 \left\{ \ln \frac{\tilde{\omega}}{T^*} + \frac{1}{\pi^2} \ln^2 \frac{T^*}{T} \right\}. \quad (9)$$

The terms coming from the remote regions in (8) and (9) play the role of renormalizations that increase the effective coupling constant, but the connection between the latter and the nonrenormalized constants is expressed by a system of parquet equations.<sup>[17]</sup> The nonrenormalized interactions themselves are, generally speaking, of the order of unity and more, since the Fermi surface reaches the boundaries of the Brillouin zone. The fact that the electrons pertain to the  $d$  band also increases appreciably the dimensionless deformation potential. In the calculations<sup>[18]</sup> for  $\text{V}_3\text{Ga}$ , the band of the structure considered above was obtained numerically ( $\sigma$  band); the calculation accuracy (2 mRy in the band structure and  $\sim 1$  eV in the relative position of the bands) does not contradict our picture. From the splitting of the terms on the edge of the cube ( $\Delta E_M \approx \sqrt{\lambda/2} \Delta E_T$ ) we obtain  $\lambda = 1/80$  and  $T^* \approx 300$  °K.

The state density in the  $\sigma$  band<sup>[18]</sup> is smaller by a factor 5–8 than that obtained from calorimetric measurements. The effective mass, however, increases

strongly when the interactions are taken into account, and this effect should evidently decrease also the value of  $T^*$ . There are still no appropriate calculations.

We note in conclusion that the logarithmic relations in (6)–(9) are sensitive to the position of  $\mu$  (i.e., to doping and strains) and to scattering effects, in agreement with the experimental situation.

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