Scientific session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the Academy of Sciences of the USSR (30 September–1 October 1987)

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A joint scientific session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the Academy of Sciences of the USSR was held at the S. I. Vavilov Institute of Physical Problems on 30 September and 1 October 1987. The following reports were presented at the session:

September 30

1. *L. P. Gor'kov.* Present state of research on high-temperature superconductivity.
2. Discussion.

October 1

3. *M. I. Katsnel'son and A. V. Trefilov.* Electron state density and anomalies in the electronic and lattice properties of metals and alloys.
4. *V. I. Antropov, V. G. Vaks, M. I. Katsnel'son, V. G. Koreshkov, A. I. Likhtenshteĭn, and A. V. Trefilov.* Effect of proximity of the Fermi level to singular points in the band structure on the kinetic and lattice properties of metals and alloys.

Two of these reports are summarized below.

M. I. Katsnel'son and A. V. Trefilov. *Electron state density and anomalies in the electronic and lattice properties of metals and alloys.* For twenty years we have been observing an anomalous behavior in many physical properties of entire classes of materials: compounds with the A15 structure, Chevrel and Laves phases, cerium and uranium compounds, carbides and nitrides of transition metals, many disordered alloys, etc. These "anomalies" are abrupt changes in properties in a narrow interval of values of some external parameter (concentration, strain, etc.). A general feature of the electronic structure of these substances is the presence of narrow peaks in the electron state density $N(E)$ near the Fermi level E_F, of a one-electron or multielectron nature. In most of the papers which have offered explanations for the anomalies in the electronic properties alone, it has been assumed that the narrow peaks are at E_F within the thermal spreading, i.e., within a few hundredths of 1 eV. This strong assumption is not actually necessary, and in certain cases it contradicts experiments or band-structure calculations. The narrow peaks, and in general any structural features in $N(E)$, can "act at a distance" of at least some tenths of 1 eV from E_F. In the lattice properties (e.g., in the elastic modulus C_{ik}) this effect is sometimes explained even in the one-electron approximation, as follows from band-structure and pseudopotential calculations for pure metals (see the following summary of the report by V.P. Antropov *et al.*). In addition, there is a universal multielectron mechanism which mediates an "action of narrow peaks at a distance" in the electronic and lattice properties: dynamic-screening anomalies. As the narrow peaks approach E_F, the contribution of the corresponding virtual transitions to the permittivity increases. This permittivity determines the effective interaction between the quasiparticles at the Fermi surface, which in turn directly determines the thermodynamic and kinetic properties.

A dynamic-screening anomaly leads to a decrease in the jump (Z) in the distribution function at E_F and, correspondingly, an increase in the effective mass $m^* \sim Z^{-1}$ and in the electron specific heat as the distance (Δ) from the narrow peak to E_F decreases. Although Z does not appear directly in C_{ik} or the magnetic susceptibility ξ, the latter may also have anomalies: C_{ik} decreases with decreasing Δ if the relation $\partial\Delta/\partial\gamma_i \neq 0$ holds (γ_i is the corresponding strain), and ξ increases as a result of an increase in the Stoner exchange amplification S if the narrow peak is associated with a local magnetic moment. In such cases, $C_{ik}(T)$ goes through a minimum, and $\chi(T)$ goes through a maximum, at $T_m \approx 0.3\Delta$ (see also Fig. 1). If Δ is sensitive to a change in volume, the bulk modulus B will have an anomaly (as it does, for example, in $Zr_{1-x}Hf_xV_2$, $CeBe_{13}$, and other cerium compounds). If it is sensitive to one of the shear strains, there will be an anomaly in the corresponding shear modulus C_{ik} (e.g., C_{44} in Zr–Nb alloys). The same (qualitative) be-

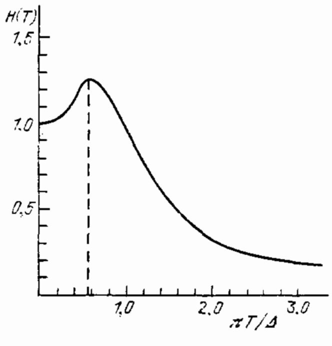

FIG. 1. Temperature dependence of the singular contributions to the elastic moduli, $\delta C_{ik}(T)/|\delta C_{ik}(0)| = -H(T)$, and to the magnetic susceptibility, $\delta\chi(T)/|\delta\chi(0)| = H(T)$, in the case in which occupied and vacant peaks in $N(E)$ close on each other. Here Δ is the distance between the peaks.

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havior results from one-particle effects associated with a narrow peak. The dynamic-screening anomalies lead to a broadening of the region of anomalies, an amplification of these anomalies, and a shift of T_m down the temperature scale. When occupied and vacant narrow peaks close on each other (the "two-peak situation"), these effects are intensified by a factor of nearly E_F/Δ. As an example illustrating the increase in S due to dynamic-screening anomalies we can cite the system $Pd_{1-x}Fe_x$ (a two-peak situation), in which ferromagnetism arises at values of x far smaller than in $Pd_{1-x}Ni_x$ (a single-peak situation).

A dynamic-screening anomaly leads to anomalies in the temperature and concentration dependence of the thermal expansion coefficient α in, for example, cerium and uranium compounds. It may be that the Invar anomalies do not result directly from a magnetic contribution to α and instead result from an influence of magnetic ordering on the position of a narrow peak.

The anomalies which we have been discussing here are not suppressed by scattering by a static disorder [if we put aide the effect of this scatttering on $N(E)$], so they can be observed as the narrow peak spreads out in disordered alloys and amorphous and liquid metals. Another feature of these anomalies which distinguishes them from electronic topological transitions is their double-sided nature to the extent that the narrow peak is symmetric.

As a narrow peak approaches E_F, there is a softening of the phonon spectra; anharmonic contributions increase; and there is an increased tendency toward a structural instability. The effect of impurities on the temperature of the martensitic transition in NiTi can be explained by band-structure calculations, which demonstrate a change in a narrow peak upon doping. A proximity of a narrow peak to E_F may lead to a negative anharmonic contribution to the lattice specific heat, as observed experimentally, e.g., in V_3Si and V_3Ga. Excitations (including phonons) with frequencies $\omega \gtrsim \Delta$ may undergo strong damping because of dynamic-screening anomalies. This effect could also explain the giant broadening of local excitations of f ions in $CeAl_3$.

Narrow peaks influence the superconducting transition temperature T_c: 1) They increase T_c because of the direct effect of virtual transitions (the Geĭlikman mechanism). 2) They increase T_c because of the softening of the phonon spectra. 3) At large values of S, they may reduce T_c because of an increase in the paramagnon suppression. The known correlation between high values of T_c and a structural instability may be related to the circumstance that the two phenomena are caused by the same factor: a proximity of a narrow peak to E_F.

In summary, a calculation of $N(E)$ upon changes in external parameters is an effective tool for studying the anomalies in the properties of materials.

[1] M. I. Katsnel'son and A. V. Trefilov, Pis'ma Zh. Eksp. Teor. Fiz. **40**, 303 (1984) [JETP Lett. **40**, 1092 (1984)]; **42**, 393 (1985) [**42**, 485 (1985)]; Phys. Lett. **A109**, 109 (1985).

[2] S. V. Vonsovskiĭ, M. I. Katsnel'son, and A. V. Trefilov, J. Magn. Magn. Mater. **61**, 83 (1986).

[3] V. I. Anisimov, M. I. Katsnel'son, A. I. Likhtenshteĭn, and A. V. Trefilov, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 285 (1987) [JETP Lett. **45**, 357 (1987)].