

# Scientific session of the General Physics and Astronomy and the Division of Nuclear Physics, Academy of Sciences of the USSR (28–29 April 1982)

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A joint scientific session of the Division of General Physics and Astronomy and the Division of Nuclear Physics of the USSR Academy of Sciences was held at the P. N. Lebedev Physics Institute of the USSR Academy of Sciences on 28 and 29 April 1982. The following papers were presented:

April 28

1. D. I. Khomskii, Electron phase transitions and the intermediate-valence problem.
2. B. I. Ivlev and N. B. Kopnin, Theory of resistive states in narrow superconductive channels.

3. K. B. Efetov, Field-theory description of Anderson localization and the conductivity of two-dimensional disordered metals.

April 29

4. N. F. Shul'ga, Development of electrodynamic processes in space and time at high energy.
5. Yu. L. Sokolov and V. P. Yakovlev, Measurement of the Lamb shift in the hydrogen atom.

We publish below brief contents of the papers.

D. I. Khomskii. *Electron phase transitions and the intermediate-valence problem.* The specific class of rare-earth compounds in which the f-level lies above the metal Fermi level or at the bottom of the semiconductor conduction band has recently been attracting a great deal of attention. A number of unique phenomena is observed in such systems. First of all, the relative positions of the f-level and the conduction band may be changed by external pressure, alloying, temperature, etc. If the f-level crosses the Fermi level or the bottom of the conduction band, an electron phase transition occurs in the system: some of the electrons transfer from it to the conduction band. There is usually no change in lattice symmetry when this happens, but the specific volume changes, the localized magnetic moment of the f-electron vanishes, conductivity changes (in particular, a dielectric-to-metal transition may occur), and other properties also experience anomalies.

In the most interesting effect, the f-level usually remains near the Fermi level after the transition (see figure), so that the average filling of this level is non-integral. This state is known as the intermediate-valence (IV) state. States with IV are characterized by a narrow resonance directly at the Fermi level  $\varepsilon_F$  (a

blurred f-level  $E_f \approx \varepsilon_F$ ) or a density-of-states peak with a width  $\Gamma \approx 10^{-2} - 10^{-3}$  eV; the concentration of these resonant levels is high,  $\geq 10^{22}$  cm<sup>-3</sup>. It is this that produces the extremely strong anomalies of practically all properties of compounds with IV (for details see the reviews in Refs. 1–3).

Two problems arise in theoretical analysis of these phenomena. The first is description of the phase transition with a change in valence: its nature (continuous, jumpwise), mechanisms, etc.; the question as to why a phase with IV always results, even on a first-order transition, is especially intriguing. The second problem area is analysis of the IV phase itself, the type of the basic compound, elementary excitations, and thermodynamic and kinetic properties.

Description is usually based on Anderson's model for magnetic impurities in a metal,<sup>4</sup> which is generalized to the concentrated case (the so-called Anderson lattice):

$$H = \sum \varepsilon_k a_{k\sigma}^{\dagger} a_{k\sigma} + E_f \sum f_{i\sigma}^{\dagger} f_{i\sigma} - \frac{U}{2} \sum f_{i\sigma}^{\dagger} f_{i\sigma}^{\dagger} f_{i-\sigma} f_{i-\sigma} + \sum (V_{ik} a_{k\sigma}^{\dagger} f_{i\sigma} + \text{H.c.}), \quad (1)$$

where  $a_{k\sigma}^{\dagger}$  and  $f_{i\sigma}^{\dagger}$  are the conduction-electron and f-electron operators, respectively; if necessary, the Coulomb interaction  $G f^{\dagger} f a^{\dagger} a$  (Falicov-Kimball model<sup>5</sup>) and the electron-lattice interaction  $g_1: f^{\dagger} f (b^{\dagger} + b) + g_2 a^{\dagger} f (b^{\dagger} + b)$  are added;  $b$  is the phonon operator.

The valence transition with a change in  $E_f$  may become a first-order transition as a result of f-s interaction or interaction with the lattice. The question as to the nature of the transition has been analyzed in many studies. For example, the importance of exciton correlations (anomalous averages of the form  $\langle a^{\dagger} f \rangle$ ) was pointed out in Ref. 6: the transition is smoothed when

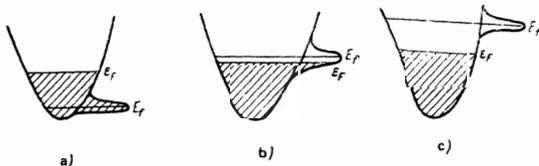


FIG. 1. Diagram of band structure in phases with variable valence (a), intermediate valence (b), and integer valence differing by one from the initial valence (c).

they are taken into account, and this stabilizes states with IV.

When, in addition to the f-s interaction, interaction with homogeneous deformation is taken into account, the first-order transition criterion takes the form<sup>7</sup>

$$2G + \left(\frac{\partial E_f}{\partial v}\right)^2 B^{-1} > \rho^{-1} + \pi\tilde{\Gamma}, \quad \tilde{\Gamma} = \pi\rho (V + G \langle a^+f \rangle)^2, \quad (2)$$

where  $B$  is the elastic modulus,  $v$  is the specific volume, and  $\rho$  is the density of states. It is found that a stepwise transition is possible here only at the expense of the lattice ( $\partial E_f/\partial v \neq 0$ ).

Allowance for local (polaron) correlations in the electron-phonon interaction also results in smearing of the transition and stabilization of the IV.<sup>8</sup> Further, by causing effective repulsion of f-electrons, interaction with shortwave phonons also stabilizes an IV phase with spatial correlations (of the Wigner-crystal type);<sup>2</sup> Coulomb repulsion of electrons by various centers also produces the same result. There would be two successive transitions in this situation: from a phase with  $n_f \approx 1$  to an IV phase with  $n_f \approx 1/2$  with superstructure, and then to phase with  $n_f \approx 0$ . However, true long-range order is improbable in the intermediate phase. Estimates indicate that the zero-point oscillations are large at realistic parameter values, and that the system is more reminiscent of a liquid with short-range order. Only if  $\Gamma/U_{\text{int}} \sim 10^{-4}$  could a "crystalline" phase result.

The most interesting unsolved problems relate to the structure and properties of the IV state itself. A simple picture of the type in Fig. 1 (virtual level or peak in density of states  $\rho(\epsilon)$  near  $\epsilon_f$ ) describes a number of the experimental results in a qualitative fashion: the high-compressibility anomaly in the IV phase, the enormous linear electronic heat capacity  $c = \gamma T$  ( $\gamma$  ranges up to  $10^3$  mJ/mole·K<sup>2</sup> the approach of the susceptibility  $\chi(T)$  to a constant value as  $T \rightarrow 0$ , etc. However, this picture cannot explain many details of the experiment. This applies in particular to the kinetic properties (conductivity, Hall effect, thermal emf, etc.). Conductivity data appear to indicate that all substances with IV can be broken down into two classes: compounds in which the ground state is purely metallic and is described by a Fermi-liquid picture, and substances of the semiconductor type. The former group includes intermetallic

compounds (CePd<sub>3</sub>, YbAl<sub>3</sub> and others), and the latter, apparently, those substances (SmS, SmB<sub>6</sub>, TmSe) that would be semiconductors in a phase with integer valence and in which all conduction electrons are electrons that have arrived from the f-level. The nature of the gap in these substances has not yet been precisely established. It may simply be of hybridization nature; however, it is much more probable that the gap is collective. For example, it might also be related to exciton effects (a state of the exciton-insulator type<sup>9</sup>).

We note in conclusion that systems with IV model, in a sense, common condensed matter consisting of electrons and ions: here f-holes play the role of heavy positively charged ions. As in ordinary systems, it is possible in principle here for a gaseous or plasma phase (integer valence,  $n_{f \text{ hole}} = 0$ ) and a condensed phase with equilibrium density  $n_{f \text{ hole}} \neq 0$  to exist; in principle, the latter could be "liquid" (short-range ordering) or "crystalline," and from the standpoint of its electron properties it may be a "metal" or a "dielectric." There is, of course, also a significant difference: here the f-electrons or f-holes and s-electrons are identical particles that are capable of turning into each other. This may result in several important consequences and greatly complicates theoretical description of these systems.

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