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ABSTRACT

The single particle and many body effects are summarized in case of 3d transition metal impurities in normal metals. It is demonstrated that two, alternative approaches give the same basic features. Impurity interaction effects are discussed both for cases with low and high Kondo temperatures. The behaviour of a regular array of 3d impurities /dilute intermetallic compounds/ in shortly described.

АННОТАЦИЯ

Обсуждаются одно- и многотельные эффекты, возникающие в случае примесей 3d переходных металлов, растворенных в простых металлах. Покажем, что два различных теоретических метода приближения приводят к идентичным результатам. Рассматриваются взаимодействия между примесями при низких и высоких температурах Кондо. Кратко описываются свойства упорядоченных 3d примесей /разбавленных интерметаллических сплавов/.

KIVONAT

Az egyszerü fémekben oldott 3d átmeneti fém szennyezések esetén fellépő egy- és többtest rezonanciákat tárgyaljuk. Kimutatjuk, hogy két, különböző elméleti megközelités lényegében ugyanolyan eredményre vezet. A szennyezések közötti kölcsönhatást tárgyaljuk alacsony és magas Kondo-hőmérsékletek esetén. A rendezetten elhelyezkedő 3d szennyezések /hig intermetallikus ötvözetek/ tulajdonságait vázoljuk röviden.

1. INTRODUCTION

Solids in which elements with unfilled 3d shell are present often show magnetic properties, this is evidenced by a large Curie-Weiss susceptibility, and possibly magnetic ordering at low temperatures. It is relatively straightforward to account for the magnetic properties in isulators, where the electrons can be taken as localized. Here the appearance of magnetic moment depends on the effective strenght of the Hund's rule, which alignes the 3d electrons parallel, and of the bonding in which electrons with antiparallel spin pairs are taking part. When bonding is weak, the resulting magnetic moment is determined by the Hund's rule, in Fe^{++} for example five of the six 3d electrons are parallel, one antiparallel, resulting in a spin $S = 2$. With strong bonding, the electrons are used up in forming chemical bonds, this gives a spin $S = 0$. The former is called a high spin, the latter a low spin configuration.

The situation is different in metals, where electrons move fast from one lattice site to another, the characteristic time, spent by one electron at a particular lattice site is given by $\tau = \hbar/\varepsilon_F$ where ε_F the Fermi energy. When ε_F is larger than the characteristic correlation energies which would keep electrons apart double occupancy of a lattice site is allowed, and only a few electrons around ε_F give rise to magnetism, which is of Pauli type in these cases. Elements with unfilled inner shells, however show

magnetism even in metal: impurities will an unfilled 4f shell show strong Curie-Weiss behaviour as a rule, and only some exeptional cases can magnetism be destroyed. This is obviously due to the fact that 4f states do not mix strongly with the host electronic states, thus electrons spend a long time on the 4f shell, and Hund's rule is effective. The mixing between 3d electrons and host is for stronger, and indeed some impurities are magnetic, while other are not. CuMn is typical of the former, CuNi or AlMn on the other hand show no obvious magnetic properties. This distinction, which depends both on the impurity, and on the host, finds it's explanation in the so called Friedel-Anderson model, the Hartree-Fock solution of which leads to a classification of dilute alloys, with sharp distinction between magnetic and non-magnetic impurities.

Obviously, a HF solution is poor for a system with such a restricted dimensionality /one scattering center embedded into a metallic host/, and strong fluctuations are smearing out the phase boundary between magnetic and non-magnetic states. Indeed, a Curie-behaviour down to T=0 occurs only if the electron at a localized level is completely decoupled from the host states, and thus has an infinite lifetime. This, however is never realized is metals, and whatever small interaction leads to a finite lifetime of the localized spin τ_s . Below $kT \sim \hbar \tau_s^{-1}$ the spin ceases to be free, and cannot be aligned easily

by the external magnetic field. This leads to a deviation from a Curie-behaviour which can be interpreted as $\mu_{\cdot H} \to 0$ as $T \to 0$, thus the impurity becomes non-magnetic at temperatures, smaller than the characteristic temperature, determined by a above lifetime effect. This transition towards a nonmagnetic state with decreasing temperature is called the Kondo-effect, and has been the subject of intensive experimental and theoretical efforts in the last decade.

Interaction effects between impurities have always played a crucial role in this field, in the dilute alloy problem the main concern was to separate properties characteristic to single impurities from "spurious" interaction effects. With the single-impurity case practically solved, interest has focused on these interaction effects, which, due to the complexity of the dilute alloy case, can give rise to broad variety of phenomena. N.Rivier is going to adress himself to the so called "spin glass" problem at this School, therefore I shall be concerned with interaction effects different from those which give rise to a random ordered magnetic systems. These are interactions between Kondo-impurities, and dilute intermetallic compounds of simple metals with 3d elements, the term dilute refers to situation where the 3d atoms are for apart, and interactions between the 3d atoms and host dominates.

2. SINGLE 3d IMPURITY IN SIMPLE METALS

2a/ Magnetic and nonmagnetic impurities

Solid solution of 3d atoms in various solvents have been studied extensively, and there is a striking correlation between the appearance of magnetism and the host properties. Also impurities in the middle of the 3d series are usually more often magnetic than those at the beginning or at the end of the series. The definition of magnetism relies on susceptibility measurements, when the susceptibility is found to be

$$\chi \sim \frac{\mu_{eff}^2}{T + \Theta}$$

the impurity is called "magnetic", a Pauli susceptibility on the other hand indicates the absence of magnetism. Table 1 shows the occurance of magnetism of 3d transition metals imbedded into various simple metals. Question marks signal banderline cases, where is of the order of room temperature, and therefore the impuritiy appears to be magnetic at high, and non-magnetic at low temperatures. It is clear from Talbe 1 that magnetism is correlated with the low electron density of the host /Au or Cu/, a higher density of host states /Al/ tends to destroy the magnetic behaviour.

Friedel-Anderson model

The explanation of this behaviour is due to Friedel /1956/ who first noticed this correlation, and explained it using scattering theory, the model which has been extensively investigated in due to Anderson /1961/, and relies also on Friedel's ideas.

The Anderson hamiltonian is written in the following form

$$H = \sum_k \varepsilon_k c_{k\sigma}^+ c_{k\sigma} + E_d^0 \sum n_\sigma + U n_\uparrow n_\downarrow + \\ + \sum (V_{kd}\, c_{k\sigma}^+ c_{d\sigma} + cc) \qquad /1/$$

The first term describes the electron states of the metallic host, the second the localized d-level of the impurity with energy E_d. The transition between the localized level and the host states is described by a transition matrix element V_{kd}, while the last term accounts for the Coulomb repulsion between electrons localized on the same 3d level. $c_{k\sigma}^+$ and $c_{d\sigma}^+$ are the creation operators of the conduction electrons and the localized d electrons with spin σ, $n_\sigma = c_{d\sigma}^+ c_{d\sigma}$ the occupation number of the localized level, U the Coulomb interaction.

In the hamiltonian /1/ orbital degeneracy is neglected*, this is probably the most serious oversimplification of

* Orbital degeneracy can probably be included by replacing U by U + 4I where I the Hund's coupling.

the model, other factors, like crystalline field splitting can probably be neglected as they are an order of magnitude smaller than the relevant energies of Eg/1/. The model cannot be solved in general, but the Hartree-Fock /HF/ solution gives a considerable insight into the problem and can also account for the absence or appearance of magnetism.

The V_{kd} interaction gives rise to a broadening of the localized d level, and the Golden rule yields a Lorentian resonance - called the virtual bound state -

$$\rho_{d\sigma}(\omega) = -\frac{1}{\pi} \frac{\Delta}{(\omega - E_{d\sigma})^2 + \Delta^2} \qquad /2/$$

$$\Delta = \pi \langle |\bar{V}_{kd}|^2 \rangle \rho_0(\epsilon_F) \qquad /3/$$

where $\bar{V}_{kd}$ is the average over k, $\rho_0(\epsilon_F)$ is the density of host states at the energy of the d-level. The occupation number of the d-level is expressed as

$$\langle n_{d\sigma} \rangle = \int_{-\infty}^{0} \rho_{d,\sigma}(\omega) d\omega = \frac{1}{\pi} \cot^{-1}\left(\frac{E_{d\sigma}}{\Delta}\right) \qquad /4/$$

In HF approximation the averaged Coulomb field shifts the d-level /but leasing it's shape unchanged/, this shift is given by

$$E_{d\sigma} = E_d^{\circ} + U \langle n_{d-\sigma} \rangle \qquad /5/$$

Inserting Eg/5/ into Eg/4/ two coupled equations are obtained

$$\langle n_{d\uparrow}\rangle = \frac{1}{\pi}\cot^{-1}\left(\frac{E_d^0 + U\langle n_{d-}\rangle}{\Delta}\right)$$

$$\langle n_{d-}\rangle = \frac{1}{\pi}\cot^{-1}\left(\frac{E_d^0 + U\langle n_{d\uparrow}\rangle}{\Delta}\right) \qquad /6/$$

Depending on E_d^0, U and Δ one has either a single solution with $\langle n_{d\uparrow}\rangle = \langle n_{d-}\rangle$, i.e. the impurity is nonmagnetic, or two symmetrical solutions with $\langle n_{d\uparrow}\rangle \neq \langle n_{d-}\rangle$ in this case the impurity is magnetic and has a net magnetic moment. Fig 1 shows the magnetic and nonmagnetic regimes as a function of $U/\pi\Delta$ and E_d/U.

The boundary is given by

$$U\,\rho_d(E_F) = 1 \qquad /7/$$

i.e. the system is more likely magnetic for larger d-states at the Fermi level.

The above HF analysis is already capable of explaining the experimental findings summaized in Table 1. The width of the d-level is proportional to the host density of states, and thus increases going from Cu to Al. A typical estimate $\Delta \sim 0.5$ eV for Cu alloys and $\Delta \sim 1\text{-}2$ eV for Al host. For Mn impurities $E_d = 0$ as the number of d electrons is five*. With Eqs/2/ and /7/ we obtain

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* With orbital degeneracy included, the total number of electrons is $2(2\ell+1)$ instead of 2, this must be included into the analysis, where for d-electrons $\ell = 2$.

$$U\rho_d(\varepsilon_F) \sim 2 \quad \text{for Cu host}$$
$$\lesssim 1 \quad \text{for Al host}$$

Nickel, on the other hand has a nearly full d-shell /$N_d = 9$/, and then from Egs/2/ and /7/

$$N\rho_d(\varepsilon_F) < 1$$

Thus, with the above parameters, the model predicts magnetic Mn impurities in Cu, but non-magnetic Mn states in Al, and also Ni should be non-magnetic in Cu /and obviously in Al/ as observed. The magnetic-nonmagnetic boundary is near Co and V for noble metal hosts, and near to Mn in aluminium, the situation in host Zn lies between these two cases.

The density of states is shown in Fig 2 for Ni and Mn impurities in Cu and for Mn impurity in Al. This behaviour has been confirmed by optical experiments, although for Au alloys the experiments are more easily understood. For AlMn the situation is not entirely clear, but the broad resonance is evident also /see for example Grüner 1974 where the optical experiments are summarized/.

The impurity resistivity can be calculated easily using the phase-shift formalism worked out by Friedel. The phase shift of the scattered electrons is given by

$$\eta_\sigma(\omega) = \cot^{-1} \frac{E_{d\sigma} - \omega}{\Delta} \qquad /8/$$

and the phase shifts obey the Friedel sum rule /charge neutrality condition/

$$N = \frac{1}{\pi} \sum_{l\sigma} (2l+1)\, \eta_{l\sigma}(E_F) \qquad /9/$$

where l the angular momentum of the scattered electrons. Retaining only the resonant phase shift $l = 2$ we obtain for the resistivity

$$R_{imp} = R_0 c \frac{5}{2} \left[\sin^2 \eta_\sigma(E_F) + \sin^2 \eta_{-\sigma}(E_F) \right] \qquad /10/$$

where $R_0 = \frac{4\pi\hbar}{e^2 k_F}$, k_F the Fermi vawe vector. The phase shifts are related to the occupation numbers of the d-states by $\sin \eta_l(E_F) = \frac{N_\sigma \pi}{5}$ in the degenerate case.

Thus going through the 3d series, the resistivity is double peaked and has a minimum when $N_\sigma \sim 5$ and $N_\sigma \sim 0$, and indeed this has been observed in Au and Cu alloys at room temperature /Fig 3/. In Al-alloys, however only a single peak is observed in the resistivity, this is taken as evidence for the nonmagnetic behaviour of 3d impurities in Al, in this case $\eta_\sigma(E_F) = \eta_{-\sigma}(E_F)$, and the peak occurs at $N_\sigma = N_{-\sigma} = 5/2$. /The shift toward smaller N values can be explained by non-resonant phase shifts η_0 and η_1 /.

Similarly other quantities, like the thermoelectric power

$$S_{imp} = \frac{\pi}{3} \frac{k_B^2}{e} \frac{T}{2\Delta} \left(\sin^2 \eta_\sigma(\varepsilon_F) + \sin 2\eta_\sigma(\varepsilon_F) \right) \qquad /11/$$

and specific heat coefficient

$$\gamma_{imp} = \frac{3\pi^2}{2} k_B^2 \left(\rho_{d\sigma}(\varepsilon_F) + \rho_{d-\sigma}(\varepsilon_F) \right) \qquad /12/$$

can be explained by the HF solution, although in some cases a larger density of states $\rho_d(\varepsilon_F)$ and smaller width Δ is obtained, than that usual, this will be discussed later.

s-d exchange model

When the impurity is strongly magnetic /CuMn for example/ it is probably adeguate to neglect all the complications coming from the potential scattering, and one can regard the impurity spin as a well defined quantity /with infinite lifetime/ which interacts with the conduction electrons, through a Heisenberg interaction. Thus the hamiltonian is given by

$$H_{sd} = 2 J(r) S_{imp} s \qquad /13/$$

where s the spin of the conduction electrons. The main contribution to J comes from the admixture of the d and s states, already considered in the Anderson model, it is

not surprizing therefore that J can be given in terms of the Anderson parameters V_{kd}, U and $E_{d\sigma}$. This correspondance has been first given by Schrieffer and Wolff in 1966 using a canonical transformation. It is, perhaps, however more instructive to derive this relation in an other way, by calculating some physical quantity in the framwork of both models.

The well known Ruderman-Kittel-Kasuya-Toshida spin perturbation around magnetic impurities can be derived using the s-d model, and we obtain

$$\sigma(r) = -\rho_0(\varepsilon_F)\,\frac{J}{8\pi}\,\frac{\cos 2k_F r}{r^3} \qquad /14/$$

This perturbation can also be given in terms of the Anderson model, in this case it is given by the difference of the charge perturbations for spin up and spin down conduction electrons. The charge perturbation is given by

$$\rho^{\sigma}(r) = \frac{-1}{4\pi^2}\,\sin\eta_\sigma\,\frac{\cos 2k_F r + \eta_\sigma}{r^3} \qquad /15/$$

and the resulting spin perturbation

$$\sigma(r) = \rho^{\uparrow}(r) - \rho^{\downarrow}(r) \approx \frac{\alpha}{4\pi^2}\,\frac{\cos 2k_F r + \phi}{r^3} \quad \text{with}$$

$$\alpha\cos\phi = \sin\eta_\uparrow\cos\eta_\uparrow - \sin\eta_\downarrow\cos\eta_\downarrow \qquad /16/$$

$$\alpha\sin\phi = \sin^2\eta_\uparrow - \sin^2\eta_\downarrow$$

Comparing Eg/14/ with Eg/16/ we obtain

$$J = \frac{2(\eta_\downarrow + (\pi - \eta_\uparrow)}{\pi \rho_0(\varepsilon_F)} = \frac{2|V_{kd}|^2 U}{E_d (E_d + U)} \qquad /17/$$

the Schrieffer-Wolff result. Eg/17/ is valid for U and $E_d \gg \Delta$, i.e. for strongly magnetic cases.

The spin perturbation can be measured by local methods, particularly by nuclear magnetic resonance /NMR/. In metals the NMR line is shifted when compared with the NMR line observed in /nonmagnetic/ insulators, this shift /called Knight shift/ arises from the coupling between the nucleus and conduction electrons. The spin perturbation around the impurities gives rise to a distribution of Knight shifts, and thus broadens the NMR signal; the broadening is proportional to c and H. By appropriate line shape analysis, and by using Eg/14/ J can be evaluated. Cu has a nucleus appropriate for NMR studies, and the J values for various impurities are shown in Fig 6. J has a minimum in the middle of the series, and increases with increasing or decreasing occupation numbers N_d, this is in accordance with the Schrieffer-Wolff result, Eg/17/. It must be noted, that due to the orbital degeneracy J measured by NMR is five times larger than J obtained by other methods.

The impurity resistivity can be obtained by using the "golden rule", and it is given by

$$R_{\text{non flip}} = J^2 \frac{S(S+1)}{3} R_0 c \qquad /18/$$

for spin conserving scattering, the spin flip scattering gives

$$R_{spin\ flip} = J^2 \frac{2S(S+1)}{3} R_0 c \qquad /19/$$

i.e. twice the value obtained for non spin flip scattering. The total resistivity is given by

$$R_{imp} = R_0 c \; J^2 S(S+1) \qquad /20/$$

With the J values determined by NMR before, R_{imp} is smallest in the middle of the series and increases again by increasing on decreasing N , in accordance with that shown in Fig 5. It is worthwile to mention that the HF expression Eg/10/ gives /using the Schrieffer-Wolff transformation, Eg/17// a value for R_{imp} which agrees with the non spin flip part. This result is the consequence of the HF approach: the spin up and spin down scattering channels are treated separately: thus no spin flip is involved.

Turning, finally, back to the magnetic properties, the magnetization is found to be reduced from the free spin value S , this is due to the antiparallel polarization of the host electron states. The reduction is given by

$$S_{imp} = S\left[1 - (2l+1)\, J\, \rho_0(\varepsilon_F)\right] \qquad /21/$$

in the s-d model. In the Anderson model, for finite the

lover resonant state is not completely filled, the upper not entirely empty and thus

$$S_{imp} = \frac{5}{\pi}\left[\eta_\sigma(\varepsilon_F) - \eta_{-\sigma}(\varepsilon_F)\right] \qquad /22/$$

is smaller than that for $u \to \infty$. Again the Schrieffer-Wolff transformation connects the effective moments obtained from the two models.

The HF solution of the Anderson model is therefore succesful in describing the main experimental results, and gives a sound theoretical basis for classifying alloys into magnetic and nonmagnetic cases, and explains why CuMn is magnetic while CuNi or AlMn not. For strongly magnetic cases it can be transformed to the s-d exchange model, which treats the impurity as a well defined spin which is weakly coupled to the host electron states. Both models are appropriate in this limit, when spin flip is properly included.

According to the HF solution, the impurities either give rise to a Curie-behaviour /$\Theta = 0$/ or to Pauli paramagnetism, but cannot explain the finite Curie-constants. In fact the susceptibility is given by

$$\chi \sim (T + \Theta)^{-1} \qquad /23/$$

and for most cases Θ is not small, and can be of the or-

der of room temperature, AuV is a typical example. Θ arises not from impurity-impurity interactions, but should be the consequence of coupling between the impurity and host.

Also, some impurities which are classified as "non-magnetic" in this sheme show large specific heats or thermoelectric powers, and a straightforward analysis, using Egs/11/ and /12/ gives a large density of states $\rho_d(\varepsilon_F)$, or small width . This enhancement of various physical quantities is also beyond the reach of the HF solution.

Impovements can be made either using the s-d model and to calculate scattering processes beyond the second Born approximation - this has been calculated first by Kondo in 1964, the name Kondo problem derives from here. One may also start from the nonmagnetic limit, and instead of HF to use RPA, this procedure has been applied by several groups, but perhaps - in case of Anderson model - first by Rivier and Zuckermann. This approach is called the localized spin fluctuation /LSF/ theory.

2b/ The magnetic-nonmagnetic transition

The Kondo-problem

It is well known since the early sixties that dilute alloys in which the impurity is magnetic have a minimum in the resistivity at low temperatures, and below the minimum the resistivity goes like

$$R_{imp}(T) \sim \ln T \qquad /24/$$

this behaviour is demonstrated in case of CuMn in Fig 6. The phenomenon remained unexplained until 1964 when Kondo first calculated the conductivity up to second order in the spin flip scattering. In the intermediate state two possibilities occur

a/ The electron with momentum K is scattered into the intermediate state with k", and this is followed by the scattering into the final state with k'

b/ An electron hole pair is created first, and then the hole annihilates the electron with momentum K. The two processes are shown in Fig 7.

In both cases the scattering rates contain the factor

$$\sum_{\varepsilon''} \frac{f_{k''}\, \rho_0(\varepsilon_{k''})}{E_{k''} - E_k} \qquad /25/$$

where $f_{k''}$ is the Fermi-Dirac distribution factor. The spin

flip scattering contributes a factor S_+S_- in the first and S_-S_+ in the second case, and thus the total scattering rate is given by

$$J^2(S_+S_- - S_-S_+)\sum_{k''}\frac{f_{k''}\,\rho_0(\varepsilon_{k''})}{E_{k''}-E_k} \qquad /26/$$

the integral diverges at $T \to 0$ or $\varepsilon \to 0$. For $\varepsilon = 0$ the temperature dependence, assuming

$$\rho_0(\varepsilon) = \begin{cases} \rho_0 & \text{if } -D < \varepsilon < D \\ 0 & \text{otherwise} \end{cases}$$

is given by

$$R_{imp} \sim 1 + \rho_0 \ln\left(\frac{kT}{D}\right) \qquad /27/$$

in accordance with the experimental observation. This surprising result is the consequence of the Fermi statistics of the conduction electrons, and of the non-commutation of the spin operators /for classical spins the spin commutator vanishes/. The impurity has an internal degree of freedom /ths spin can be either up or down/ and this provides a coupling between electrons scattered succesively on the impurity. Unlike in case of potential scattering, to total scattering process cannot be separated into independent scattering events.

Naturally a diverging resistivity cannot be a real solution of the problem, as R_{imp} should saturate at low temperatures as it cannot exceed the maximum scattering, given

by the phase shift $\pi/2$. Following calculations, performed by Abrikosov and Suhl included all leading logarithmic terms, as it is expected that they also contribute heavity to the resistivity. Instead however of removing the singularity, the solution diverges not only at T = 0, but at finite temperature, which is given by

$$T_K = \frac{\varepsilon_F}{k_B} \exp\left[-1/J\, \rho_0(\varepsilon_F)\right] \qquad /28/$$

the behaviour of the resistivity for the Kondo- and Abrikosov-Suhl approach is given in Fig 8. Clearly, T_K defined above is not the temperature below which the state of the impurity should be modified drastically by the interaction of the conduction electrons.

The so called Kondo temperature T_K depends exponentially on the s-d coupling J, and looking at Fig 5, where J is plotted across the 3d series for Cu, it is evident, that T_K can range from the mK region up to well above room temperature. Fig 9 shows T_K determined on experimental grounds /discussed below/ for Au, Cu /and also for Al-based alloys which will be discussed later/. The exponential dependence of T_K on J is convincingly demonstrated by Fig 9.

Subsequent theoretical approaches /equation of notion method, dispersion relations and summation of wider class

of diagrams/ have removed the spurious singularity and resulted in a e.g. finite resistivity at T = 0. The discussion of these approaches and the correspondance between them is beyond the limit of the present note, I shall merely concentrate on the behaviour of various physical quantities by going through T_K, and to discuss the general behaviours at low temperatures $T \ll T_K$.

Temperature dependences of various physical quantities

It has already been mentioned, that the susceptibility does not obey a straightforward Curie-law but a finite θ value appears, usually θ is the measure of T_K in dilute alloys. Alternatively, the susceptibility can be written as

$$\chi(T) = \frac{\mu_{eff}^2(T)}{3k_B T} \qquad /29/$$

and then the effective moment gradually disappears below the Kondo temperature. The specific heat has a hump at around T_K, the total entropy is given by

$$\Delta S = \int_0^\infty \frac{C_v(T)}{T} dT = R \ln(2S+1) \qquad /30/$$

indicating that the spin entropy is removed from the system below the Kondo temperature. The resistivity increases logarithmically above T_K, then changes slope at around the Kondo temperature and saturates at the unitarity limit at low temperatures. The behaviour of the susceptibility, specific heat and transport properties is sketched in Fig 10.

It should be emphasized that all the various physical quantities are in accordance with those calculated by impoved methods, but the approximations progressively break down when going below T_K. The experimental situation has also be cleared up only recently, mainly due to the fact, that impurity-interactions play a more and more important role at low temperatures. It appears, however, that by now we have achieved a unified picture on properties well below T_K.

Properties at $T \ll T_K$

In contrast to the logarithmic dependences well above the condo temperatures, the various physical quantities are given by simple power laws of the temperature well below T_K. Thus

$$R_{imp}(T) = R_{imp}(0)\left[1 - \frac{\pi^2 k_B^2 T}{6\Gamma^2}\right] \qquad /31/$$

where $R_{imp}(T=0)$ is the unitarity limit resistivity determined by the charge neutrality, assuming $\eta_\sigma(\varepsilon_F) = \eta_{-\sigma}(\varepsilon_F)$. The specific heat

$$C^V_{imp} = \frac{2(2l+1)\pi k_B^2 T}{3}\left[1 - \frac{\pi^2 k_B^2 T}{\Gamma^2}\right] \qquad /32/$$

the susceptibility

$$\chi(T) = \frac{2(2l+1)\mu_B^2}{\pi\Gamma}\left[1 - \frac{\pi^2 k_B^2 T^2}{3\Gamma^2}\right] \qquad /33/$$

and the thermoelectric power is proportional to the temperature /but influenced also by the potential scattering/.

In all cases Γ is a characteristic energy and is of the order of the Kondo energy $k T_K$. The detailed analysis of the various physical quantities gives nearly identical values, for CuFe $\Gamma \sim 0.2 \times 10^{-2}$ eV, for AuV $\Gamma \sim 2 \times 10^{-2}$ eV. In fact, usually $\Gamma = k T_K$ is defined, this, together with - for example - the θ value determined from the high temperature susceptibility provides the T_K values given in Fig 9.

The most important factor probably is, that the temperature dependences given by Egs/31/-/33/ are identical to that obtained from the standard Sommerfeld expansion, suggesting strongly that a Fermi-liquid type behaviour is realized well below the Kondo temperature. The effective width appearing in the expansion Γ, can be taken as the width of the many-body resonance which appears at ε_F as a consequence of the strong coupling of the conduction electrons through the impurity.

This narrow resonance - called usually the Abrikosov--Suhl resonance - appears most probably together with the single-particle resonances /the split resonances appropriate for the magnetic limit of the Anderson model/ as the latter provide the background for the s-d model itself.

Naturally, it is desirable to find an experimental technique, which provides a direct measure of the narrow many body resonance. Unfortunately optical experiments do

not work near ε_F and therefore cannot give valuable information in this respect. The measurement of the correlation effects near to the impurity, in principle, should provide with such a tool. The case in point is as follows: a strongly energy dependent scattering is expected to have a drastic influence also for away in space. One can define a coherence length

$$\xi = \frac{v_F}{2\Gamma'} \qquad /34/$$

where v_F is the Fermi velocity, Γ' the overall energy dependence of the scattering. The various correlation functions are expacted to be modified for $r < \xi$. We note that for $T_K \sim 10^oK$, $\xi \sim 10^4$ Å !

This coherence effect is expected to show up in the charge perturbation around the impurities. It has been demonstrated to exist in AlMn, but unfortunately for real Kondo systems like CuFe relevant experiments have not been performed yet. Also, spin correlation functions, measured by neutron scattering should indicate the strong modification at distances smaller than ξ , but again, the experimental situation is not clear enough to arrive at a definite conclusion. It appears experimentally, that this effect does not show up in the spin polarization itself, recent careful NMR experiments reveal no correlation effects. Wheather the effect on the polarization is expected or not is still disputed, therefore these experiments are also not decisive in this respect.

Nevertheless, our present understanding of the Kondo problem suggest a strong renormalization of the effective coupling between the impurity spin and conduction electrons below the Kondo temperature T_K. The magnetization of the impurity + conduction electrons disappears as $T \to 0$ and the susceptibility remains finite at T=0. As a consequence of this renormalization a many-body resonance appears at ε_F, which has a Lorentzian top and logarithmic tail, this leads to spectacular changeover from logarithmic dependences above T_K to Fermi liquid behaviour below T_K, the transition between the two regions is smeared out by the strong fluctuations due to the low dimensionality. The single-particle /Friedel--Anderson/ resonances still appear at higher energies, thus the density of states looks like shown shematically in Fig 11, but do not play an important role in the Kondo-problem which is determined by processes at $K T_K$ near ε_F.

Not surprizingly, the renormalization group method applied by Wilson to the Kondo problem leads to e.g. a susceptibility in full accord with the experiments, and can most probably regarded as a final solution of this exciting field of solid state physics.

LOCALIZED SPIN FLUCTUATIONS

It has been mentioned before, that the HF analysis of the Anderson model anderestimates the width Δ of the virtual bound state in some cases, where the parameters u and $\rho_d(E_F)$ indicate that the system is near to the magnetic--nonmagnetic boundary; typical examples for this are AuV or AlMn. One observes a large specific heat, a large thermoelectric power, and also a susceptibility which is larger than that would correspond to a Pauli susceptibility, with density of states $\rho_d(E_F)$ obtained from the HF analysis. The measured quantities thus are enhanced, and indicate a larger effective density of states at the Fermi level. Also in case of AlMn, elegant experiments performed by Caplin and Rizzuto in 1967 demonstrated that

$$R_{imp}(T) = R_{imp}(0)\left[1 - \left(\frac{T}{\theta'}\right)^2\right] \qquad /35/$$

and analyzing this behaviour in terms of simple Sommerfeld expansion, from θ' on effective width Δ' was obtained. All different kind of macroscopic experiments give an enhancement factor $\frac{\Delta}{\Delta'} = \eta \sim 10$ for AlMn.

It seemed to be natural to attack the problem from the non-magnetic side of the Anderson model, and then it is clear that the enhancement of the various physical quantities is due to the fact that the system is being near to the magnetic boundary, in other words it is "nearly magnetic".

In the Anderson model repulsive electron-electron interactions are responsible for the appearance of magnetism, this can be represented as an attractive electron-hole interaction. In the RPA approximation, the summation of the Ladder diagram shown in Fig 12 leads to an electron--hole matrix

$$T(\omega) = \frac{1}{\pi} \frac{1}{\omega + i\tau_0} \qquad /36/$$

with

$$\tau_0^{-1} = \frac{\pi \rho_d(\varepsilon_F)}{1 - U \rho_d(\varepsilon_F)} \qquad /37/$$

τ_0 can be taken as the lifetime of the electron-hole correlations, which goes to infinity approaching the magnetic nonmagnetic boundary, hence the name of localized spin fluctuation. With the T-matrix given above one proceeds to calculate the density of states and the various thermodinamic quantities in the usual way. The self energy is given by

$$\Sigma_d(\omega) = \Sigma T \; T(i\omega_n) G_d^0(i\omega_n + \omega) \qquad /38/$$

where

$$G_d(\omega) = (\omega - E_d \pm i\Delta)^{-1} \qquad /39/$$

and then

$$G_d(\omega) = \frac{1}{\omega - E_d \pm i\Delta - \Sigma_d(\omega)} \qquad /40/$$

A large effective density of states is found by the renormalization of the Green's function, and the enhancement effects can readily explained. The basic problem with the above procedure is twofold. First of all the RPA expression diverges at the HF boundary, see Eg/36/, which is most certainly an artifact of the approximation. Thus the RPA starts to break down in region when it starts to give impoved results over the HF treatment. Secondly, although it is intuitively clear that repulsive electron-electron interactions are dominating in the magnetic properties, beside the electron-hole channel, the electron-electron channel should also be considered. This leads to enormous mathemathical complications /parguent diagrams etc/, and not surprizingly no exact treatment of the problem exist at present.

In a semiphenomenological way one may assume, that the T-matrix has the form of Eg/34/, but τ_0 is a free parameter, which can be adjusted to account for various physical quantities. This so called dominant pole approximation has been worked out in considerable detail by Zlatic and Rivier, who realized that, in spite of the fact that no relation between τ_0 and the basic parameters of the Anderson model U, E_d and Δ can be obtained, the basic properties of dilute alloys can be accounted for. τ_0^{-1} can be taken as the characteristic enhanced width, observed be experiments.

The general picture energing from this sheme is surprisingly similar to that found in the Kondo problem. The static magnetic susceptibility goes as

$$\chi(T) = \chi(0)\left[1 - \left(\frac{T}{\Theta}\right)^2\right] \qquad /41/$$

at low temperatures, and has a Curie-Weiss form above the temperatures $\hbar/\tau_0 \sim k T_C$, similarly to that found by the solution of the Kondo problem; thus T_c can be taken as the Kondo temperature.

It is perhaps most instuctive to look at the density of states obtained by the dominant pole approximation, this is shown in Fig 13 with parameters appropriate for AlMn and CuFe. One observes two broad resonances displaced symmetrically with respect to the Fermi level, and one can associate with the partially split virtual bound state - obtained in HF in the magnetic limit! In addition to the broad structures a narrow resonance appears at ε_F, which has a width τ_0^{-1} / 600°K in case of AlMn, and 30°K in case of CuFe/, and a Lorentzian top, leading to the simple power laws at low temperatures. In the Kondo problem, the narrow resonance is called the Abrikosov-Suhl resonance. It appears therefore, that the approximation may reproduce all the important features of the Kondo-problem, but starting from an entirely different point of view. The semphenomenological LSF approach can therefore produce a gemine magnetic impurity, and probably there is no basic difference between the LSF and Kondo descriptions of a localized magnetic 3d moment in simple metals.

3. IMPURITY INTERACTIONS - TOWARDS 3d METALS

The obvious way to extend our present knowledge about single 3d impurities in simple metals to treat interaction effects in random or regular systems also consisting of 3d and simple metallic elements; this approach, hopefully, leads to a better understanding of the 3d metals themselves too.

The complexity of the single impurity problem suggests, that we are facing a rather complicated situation, and in general depending on the 3d atom and on the host various types of interactions occur: impurities which have a $T_K \sim 1^oK$ should interact differently at 10^oK from those with $T_K \sim 10^{3o}K$. For random alloys, there is one well defined class of materials, which appear to have common properties, these are the alloy systems for which T_K is much less than the average interaction energy between the impurities. Each impurity can be regarded as a well defined spin, interacting with the host through the s-d interaction. Below a certain temperature, the alloy is frozen magnetically, and has rather interesting properties in the low temperature phase. This is called the spin glass state, and is the subject of Dr. Rivier's talk at this School.

Interaction between impurities, which are in the Kondo--state can - naturally - not be treated by sound theoretical

medhods, nevertheless I shall attempt to account for some features expected /and observed/ under such circumstances. Both in the spin-glass problem and in the interacting Kondo-regime the alloy is disordered, the 3d atoms are randomly arranged. It is, however, also possible to construct a periodic array of 3d atoms, which are far apart /no direct d-d overlap/ and are embedded into a metallic host. All the basic physics, contained in the Anderson model remains, but due to the periodic array of 3d scattering centers band formation is possible. This subject has been started by A.D.Caplin, and by now we have a wide range of such "dilute intermetallic compounds". The last part of the notes is concerned with the description of ideas appropriate for these materials.

Impurity interactions in Kondo system

It has been recognized a few years ago, that interactions between impurities plays a crucial role in Kondo alloys, and the smaller the Kondo temperature T_K, the smaller the critical concentration, beyond which interaction effects are evident. An empirical relation

$$c_{crit} \sim \frac{k_B T_K}{\varepsilon_F} \qquad /42/$$

was constructed to describe the experimental findings. Eg/ / is an extremely strong criterium, for CuFe for example $T_K \sim 30^{\circ}K$ and $\varepsilon_F \sim 7$ eV is of the order of 100 ppm! The appearance of the Kondo temperature in the critical

concentration suggest, that the compenzation of the impurity spin is crucial in this interaction mechanism.

Naturally C_{crit} is not a well defined quantity, there is for example no phase transition to an ordered state as it is happening in the spin glass problem. One merely observes, that the measured Kondo temperature depends on the concentration, the overall temperature dependences remain, however unchanged. The impurity resistivity, for example is given by

$$R_{imp}(T,c) \sim 1 - \left(\frac{T}{\theta(c)}\right)^2 \qquad /43/$$

with θ depending on the concentration, θ decreases with increasing c, and at low concentration it can be given by

$$\theta(c) = \theta(0) - c\,\frac{\varepsilon_F}{\partial T_K} \qquad /44/$$

Similarly to the resistivity, the specific heat and susceptibility was found also to be concentration dependent, but again the overall temperature dependences remain unchanged, in all cases simple power laws govern the T-dependences of the various physical quantities. This behaviour has been observed in a number of cases, including CuFe, AuV and AlMn, at temperatures smaller than T_K /$\sim 30^\circ$K for CuFe, $\sim 300^\circ$K for AuV and $\sim 600^\circ$K for AlMn/.

The effect should be sharply distinguished from that observed at temperatures $T \gg T_K$ where the impurities have a well defined spin, in the latter case the concentration dependences are different, and what is more important, the various transport, thermal and magnetic properties behave in a completely different way.

It is essential to account for the general behaviour described above by looking at the properies of the impurity + conduction electron system in the Kondo state $T < T_K$. The many body screening of the impurity spin is essential in this temperature region. Conduction electrons at energy range kT_K around ϵ_F are performing the Kondo screening, the wave function of each electron is modified in this energy range. Thus to screen one impurity with spin S-1/2 one needs approximately ϵ_F/kT_K conduction electrons. With increasing impurity concentration not all the impurity spins will be screened, as the number of conduction electrons is less than that required for the screening, and thus the average Kondo temperature $T_K(c)$ decreases, the rate of decrease is given by ϵ_F/kT_K, as observed. One arrives essentially to the same conclusion by observing that the Kondo screening leads to a large coherence length $\xi = \frac{v_F}{kT_K}$, and with increasing impurity concentration the coherence regions start to overlap and this leads to impurity-impurity interactions. The above explanations can be found in Star's thesis /1971/. The above arguments

can be extended to account for numerical agreement between the calculated and experimentally found concentration dependences; clearly a linear c dependence cannot be valid for higher concentrations. Using a statistical picture, T_K depends logarithmically on the concentration, this has been verified by careful analysis of relevant experimental data /Babic and Grüner 1976/.

Naturally, it is not possible to calculate the temperature dependences of the various physical quantities for an interacting Kondo system. It has, however been argued by Mott /1974/ that the Kondo process and the highly correlated electron gas have many similarities, and can be viewed as two opposite limits. In the Kondo process, one has one impurity and an infinite number of scattering electrons, in the highly correlated electron gas the number of excess electrons in few. In both cases Fermi-liquid type behaviours are observed, with enhancements of the various quantities /like specific heat, susceptibility/. In interacting Kondo system is somewhere between these two limits, it is not surprizing therefore, that here again simple power laws of temperature are observed.

It is also important to realize, that the interaction effect described above and that leading to the spin glass state are acting against each other. Broadly speaking, due to the indirect spin-spin RKKY interaction becomes weaker,

and the tendency towards a magnetically ordered state is supressed. On the other hand, the RKKY coupling between the impurities can be viewed as an internal magnetic field existing at the impurity site. The spin flip scattering thus becomes inelastic, and the Kondo effect is supressed in a similar way that that is caused by a static external magnetic field. The resulting ground state will obviously be extremely complicated, in particular for cases where the two processes just balance each other. It is however postulate a tentative phase diagram of impurity interactions, including both types of effects, this phase diagram is shown in Fig 14. With increasing impurity concentrations T_K drops, below T_K one has the collective Kondo state discussed before. By increasing a further T_K decreases to values smaller than the average RKKY interaction energy, and then the mechanism which leads to the spin glass state starts to be operative, with increasing impurity concentration a typical spin-glass state is achieved. For rather high concentration of impurities, nearest neighbour interactions are perhaps dominant, this can lead to properties different from 60th the collective Kondo, and spin glass behaviour.

The various properties, expected on the basis of Fig 14 can, naturally be observed in some favourable cases. When T_K is small, mainly a spin-glass behaviour is observed, AuFe is typical for this /$T_K \sim 1^{\circ}K$/. On the other hand when T_K is higher than room temperature, spin glass behaviour is not

observed. The collective Kondo state extends to high concentrations, where direct nearest neighbour interactions are dominating, AlMn is a typical alloy where this behaviour is observed. CuFe may be a good candidate for looking at effects discussed before, here however metallurgical effects play a crucial role, it appears that perhaps for materials where the host is a d-metal /like PdRh/ the phase diagram shown in Fig 14 is appropriate.

Dilute intermetallic compounds

In intermetallic compounds the constituent atoms are periodically arranged, the term dilute refers to situations where the 3d atoms are for apart, and then we are free from complication due to direct d-d overlap /as in 3d metals/. A hypotetical one dimensional dilute compound is shown in Fig 15. Because of the absence of d-d overlap, the d-states are broadenced by the V_{kd} interaction, similarly to the dilute alloy case, and we expect also the local Coulomb interaction to be similar. Thus the magnetic properties are determined by the same parameters as in dilute alloys, we expect therefore, that phase is a close parallelism between a dilute alloy and dilute compound.

The two systems, however differ in several important aspects. First of all, due to the periodic arrangement of the 3d atoms, the 3d states form bands, and have a well defined k -vector dependence. The resistivity should disap-

pear at T=0 for a regular array of scatterers in contrast to the random alloy case, but it is expected that fluctuation effects appear in the temperature dependences. It is also important to note, that in a dilute compounds local bonding effects can be more pronounced than in a dilute alloy, as in the former the whole crystal structure is cemented together by such local interaction; in a dilute alloy the 3d impurity sites in a /for example fcc/ symmetry determined entirely by the host.

The first systematic investigation has been performed by Caplin and Dunlop /1972/ who investigated the iso-structural compounds Zn_{13}3d, were 3d is Mn, Fe and Co. A striking correlation was found between the magnetic properties of the Zn_{13}3d phases and the corresponding Zn3d dilute alloys. Zn_{13}Mn was found to be magnetic, with effective moment 1.8/u_B /in contrast to $U_{eff} \sim 4/u_B$ found in ZnMn/. Only a rather small moment was observed in Zn_{13}Fe, and indeed Fe in Zn is also weakly magnetic. Zn_{13}Co is nonmagnetic, neither was Co found to be magnetic in a Zn host. The virtual bound state width was found to be similar in the intermetallic compounds and dilute alloys, this explains the close similarity in the magnetic properties.

The resistivity was disappearing going towards T=0 /aside some small residual resistivity/, and in the Zn_{13}Fe compound $R \cdot T^2$ at low temperatures, signalling strong fluctuation effects. The most dilute Al-3d intermetallic

compounds were investigated by Dunlop, Grüner and Caplin /1974/. The low temperature specific heats suggest a large contribution coming from the d-states, γ /mole of 3d atom is shown in Fig 16. The overall behaviour can be explained by

$$\rho_d(\varepsilon_F) = \frac{10}{\pi\Delta}\sin^2\left(\frac{\pi N_d}{10}\right)$$

where N_d varies accross the 3d series in the usual way. The virtual bound state width $\Delta \sim 2$ eV, probably somewhat larger than that expected for dilute alloys. The temperature dependence of the resistivity can also be explained by scattering from s to d states, the temperature dependences were found to be strongest in the middle of the series. None of the compounds were found to be magnetic, in the Friedel-Anderson picture this is due to the large width i.e. all the compounds are in the nonmagnetic limit. An other likely explanation - clearly outside the reach of the nondegenerate Anderson model - is that Hund's rule is not obeyed in these compounds, due to strong bonding effects /in contrast to the dilute alloy case/.

Experiments, performed on somewhat more concentrated /but still dilute in the sense described before/ compounds revealed, that the latter situation may be more appropriate in Al-based intermetallic compounds. Several compounds of Al and Mn show well defined Curie-Weiss behaviour, with small θ values and also with rather small effective moments /of around 1.8 μ_B characteristic of S=1/2/. The small

values suggest that the moments are well defined and have a long lifetime - but then in the Anderson model they should have moments near to the free ionic value, $S = 5/2$ or S=2 for Mn. The contrasting behaviour observed in Au-Mn and Al-Mn compounds is shown in Fig 17 where values are collected for several compositions. In the gold compounds the effective moments are always near to S=2, and small differences are most probably due to polarization effects. The compounds order magnetically at low temperatures, again suggesting well defined moments on the Mn sites. In contrast to this, manganase has always a small moment in Al-Mn compounds, the θ values very from compound to compound but are usually of the order of $100^{\circ}K$. The compounds do not order down to the helium temperatures.

It has been supposed by Grüner and Mott /1974/ that the transition metal ion can exist in a high spin state /Hund's rule/ and low spin state /anti Hund's rule/, and that in some cases the low spin state has a lower energy. This leads to an energy level sheme shown in Fig 18 for an atom with S=0 ground state and S=1 excited state - both have $3d^n$ electrons. The two cofigurations are separated by the $3d^{n+1}$ state lying for above in energy. The model leads to an admixture of the S=1 state, and to a long lifetime of this state due to the barrier which separates it from the ground state.

In contrast to the Kondo problem, where the spin flip scattering occurs between states having the same energy /in the absence of external magnetic field/, here we have various possibilities. Scattering from the S=0 to the S=1 state requires a finite energy and thus leads to a Kondo side band - a behaviour similar to that in case of Kondo scattering with external magnetic field. Also both in the S=0 and S=1 state Kondo effect can be operative. This leads to various possibilities, depending on the parameters of the model, the reistivity for example may show typical Kondo anomalies or may have a maximum as a function of temperature. The strong fluctuations lead to a finite lifetime of the state which has a moment, if this lifetime is short, magnetic interactions are strongly depressed, and magnetically ordered phases are not observed.

The model was found to be appropriate to describe various physical quantities of Al3d intermetallic compounds, and is particular in several respects. First of all, it assumes that Hund's and thus magnetism can is be destroyed by local /bonding/ effects. This has not been considered in metallic systems where the appearance or disappearance of magnetism depends only on the Coulomb interaction and bandwidth D in general; the crucial parameter being U/D. It indicates, that the question of Hund's rule must be rised again, in particular in cases, where other evidences for

bonding effects are found /in the crystal structures for example/. Also, the model treats fluctuations between states with the same occupation numbers, but with S=0 and S=1, this is clearly not possible in the non-degenerate Anderson model. The model is thus a rich one, but probably much more difficult to treat than the Anderson model.

CONCLUSIONS

Dilute alloys are prototypes of systems with strong many body effects. They manifest themselves is strong fluctuations, in a central peak /Abrikosov-Suhl resonance/ and long range correlation effects. Careful and systematic experimental work lead to a more ore less complete picture on the many-body and single particle effects, and there appears to be and adegnate theoretical background to account for the observed behaviours. The basic parameters of the model, which account for the main properties are the correlation energy U and virtual bound state with Δ . The question of orbital degeneracy and thus the importance of Hund's rule, has been raised several times by several workers in this field, but has only rarely been tried to invoke in various theoretical attempts. This in contrast to the general situation for 4f impurities, where Hund's rule has obviously a fundamental importance.

Impurity interactions have always played an important role, and due to the complexity of the Kondo problem itself, a broad variety of phenomena are expected, depending wheather impurities are magnetic or are in the Kondo state; the former leads to a spin glass, the latter most probably to a highly correlated electron gas. In ordered compounds the resulting crystals structures often resemble strong local configurational effects between the 3d and normal metal atoms, these can lead to situations reminiscent to insulators - i.e. high spin and low spin configurations.

While the basic aspects of the Kondo problem are being understood, the problem of impurity interactions and also the question of compatibility of Hund's rule and fermi liquid theory are challenging, with broad perspectivers for both experimental and theoretical work in this field.

TABLES

Table 1 Magnetic and nonmagnetic impurities in Au, Cu, Zn and Al matrix. The sign M and NM refers to cases where the impurity was found magnetic or nonmagnetic, question marks indicate borderline cases

FIGURES

Fig 1 Magnetic and nonmagnetic regime in the HF treatment of the Anderson model

Fig 2 Density of states obtained from the HFsolution of the Anderson model, for CuMn, CuNi and AlMn

Fig 3 Room temperature resistivities of Au and Cu alloys

Fig 4 Room temperature resistivities of Al alloys

Fig 5 J values for Cu based alloys obtained from host NMR studies

Fig 6 Resistance minimum for CuMn alloys. The concentration /in at%/ is also shown in the figure

Fig 7 Time ordered diagrams corresponding to the conduction electron scattering

Fig 8 Behaviour of the resistivity for the Kondo- and Abrikosov-Suhl approximation

Fig 9 Kondo-temperatures for 3d impurities in Au, Cu and Al host

Fig 10 Behaviour of the susceptibility X, specific heat C_v, thermoelectric power S, and resistivity R near T_K.

Fig 11 Single particle and many body resonances for a Kondo impurity below T_K.

Fig 12 Electron-hole ladder diagram considered in the RPA approximation

Fig 13 Density of states appropriate for AlMn obtained from the dominant pole approximation of the Anderson model

Fig 14 Phase diagram for impurity interactions in dilute alloys

Fig 15 One dimensional simple metal and dilute compound

Fig 16 Electronic specific heat coefficients per mole of 3d atom in Al3d compounds

Fig 17 Effective magnetic moments in Au-Mn and Al-Mn intermetallic compounds

Fig 18 Energy level sheme of a 3d atom with anti Hund's rule state having the lover energy

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Table 1

HOST / IMPURITY	Au	Cu	Zn	Al
Ti	NM	NM	NM	NM
V	?		NM	NM
Cr	M	M	M	?
Mn	M	M	M	?
Fe	M	M	M	NM
Co	?	?	NM	NM
Ni	NM	NM	NM	NM

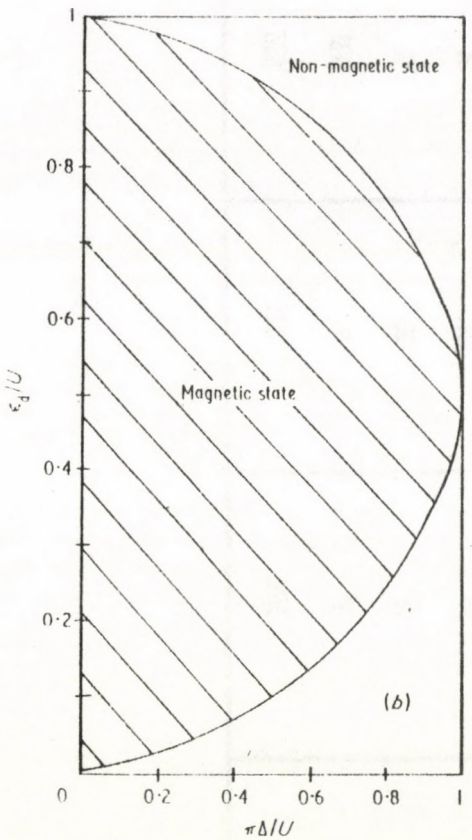

Non-magnetic state
Magnetic state
(b)
1
0·8
0·6
0·4
0·2
0
0·2
0·4
0·6
0·8
1
ε_d/U
$\pi\Delta/U$

Fig.1

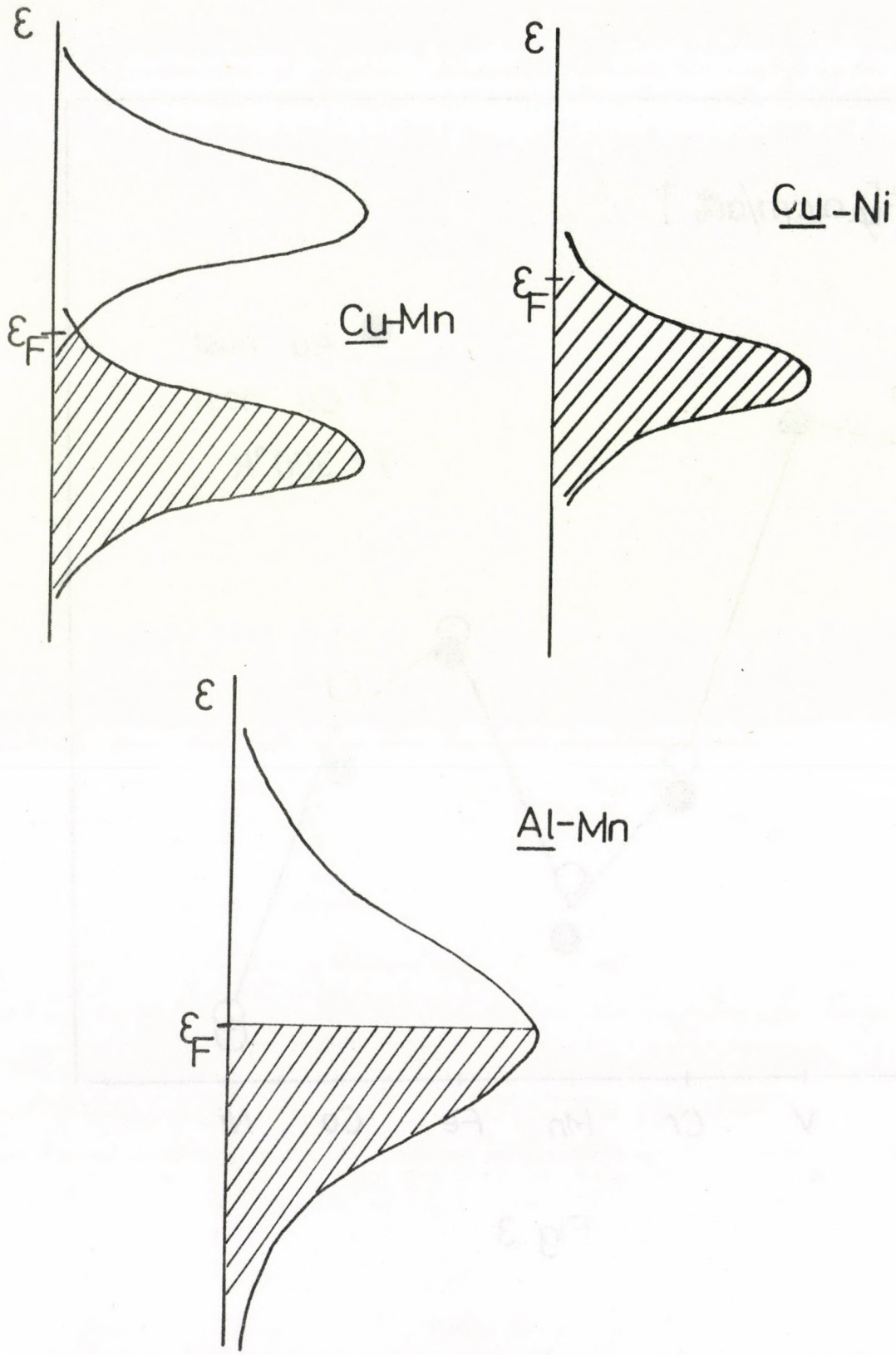


Fig. 2

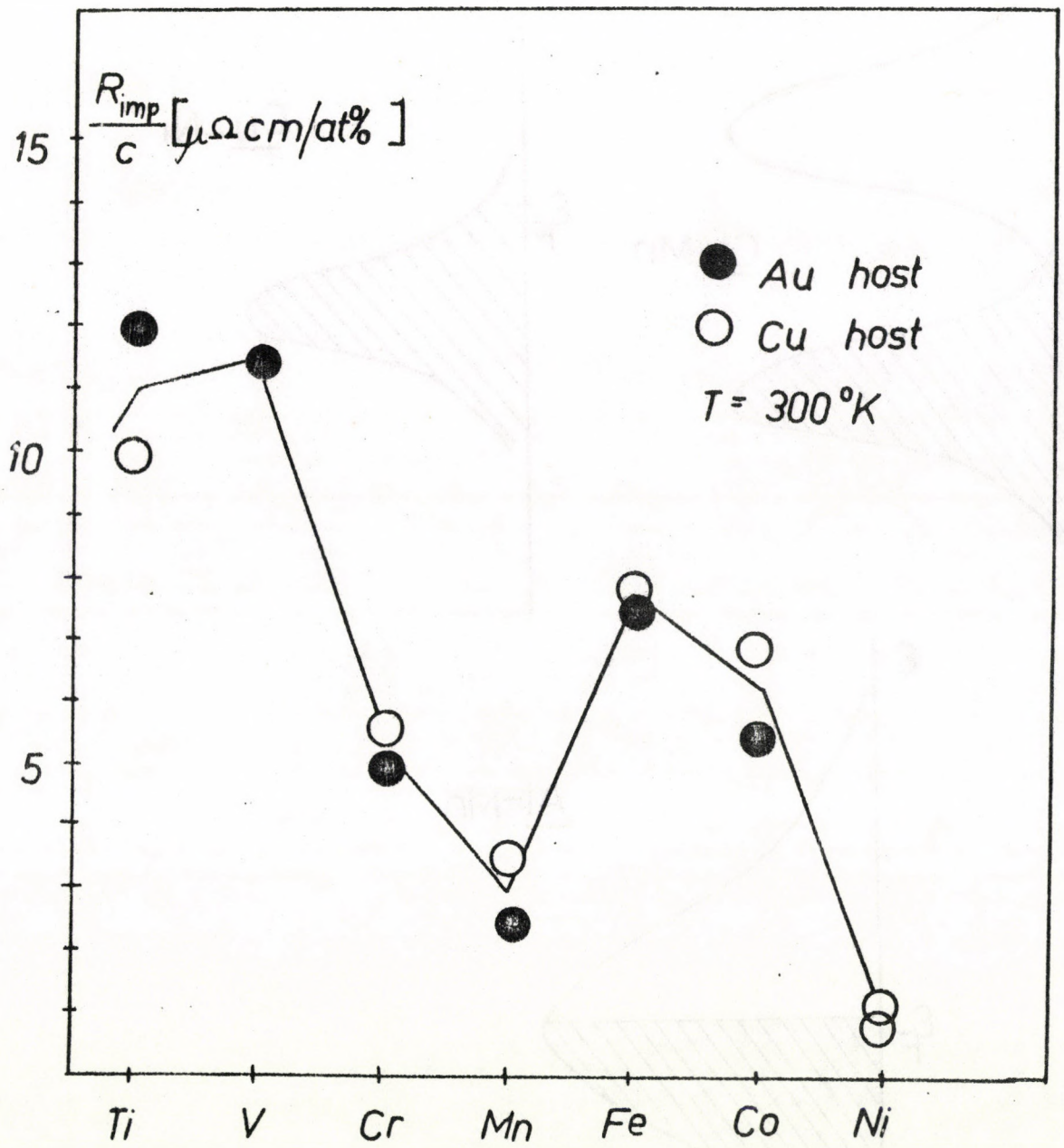

$\frac{R_{imp}}{c}$ [μΩcm/at%]
15
10
5
Au host
Cu host
T = 300°K
Ti
V
Cr
Mn
Fe
Co
Ni

Fig. 3

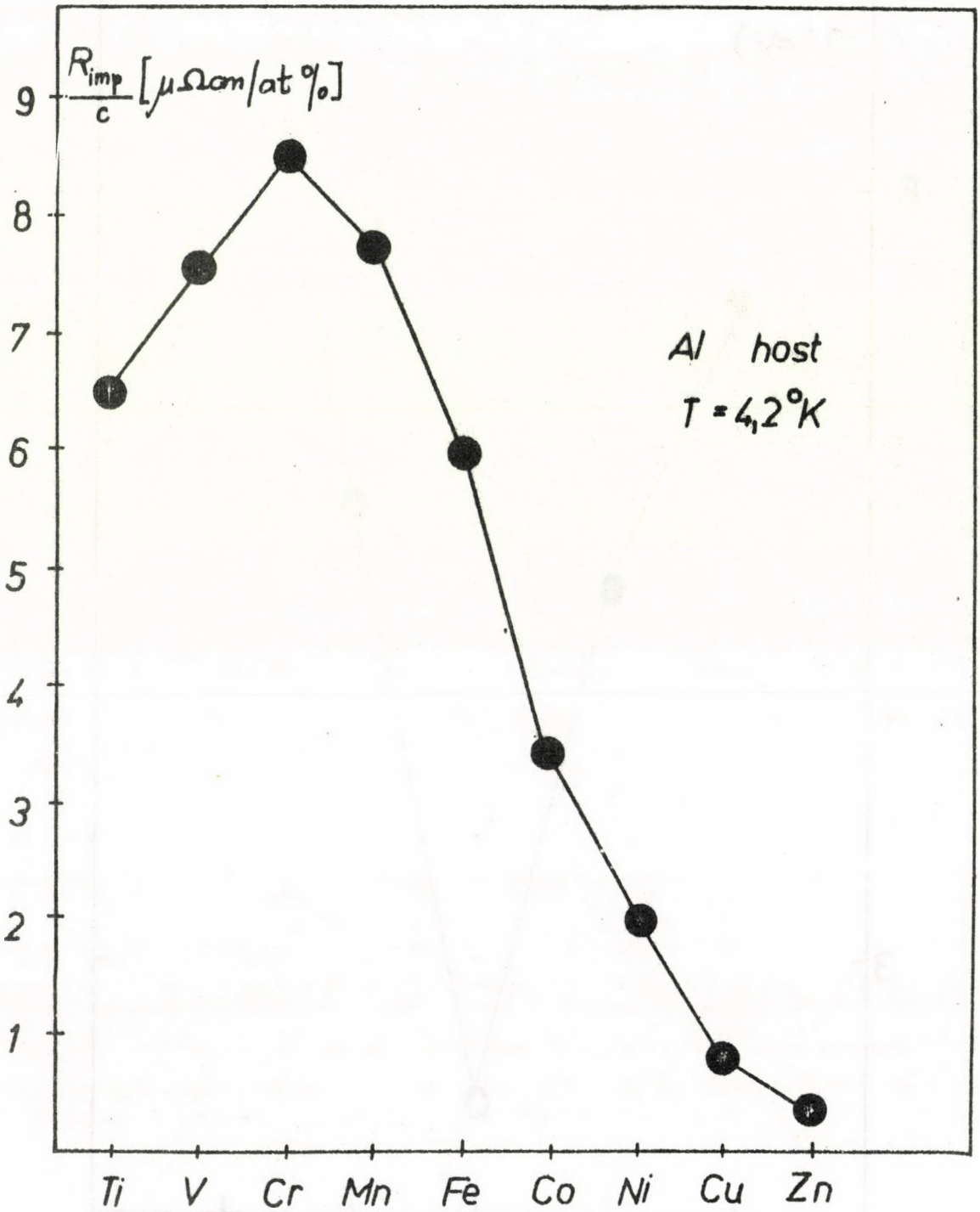

$\frac{R_{imp}}{c}$ [μΩcm/at %]
9
8
7
6
5
4
3
2
1
Al host
T = 4,2°K
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn

Fig. 4

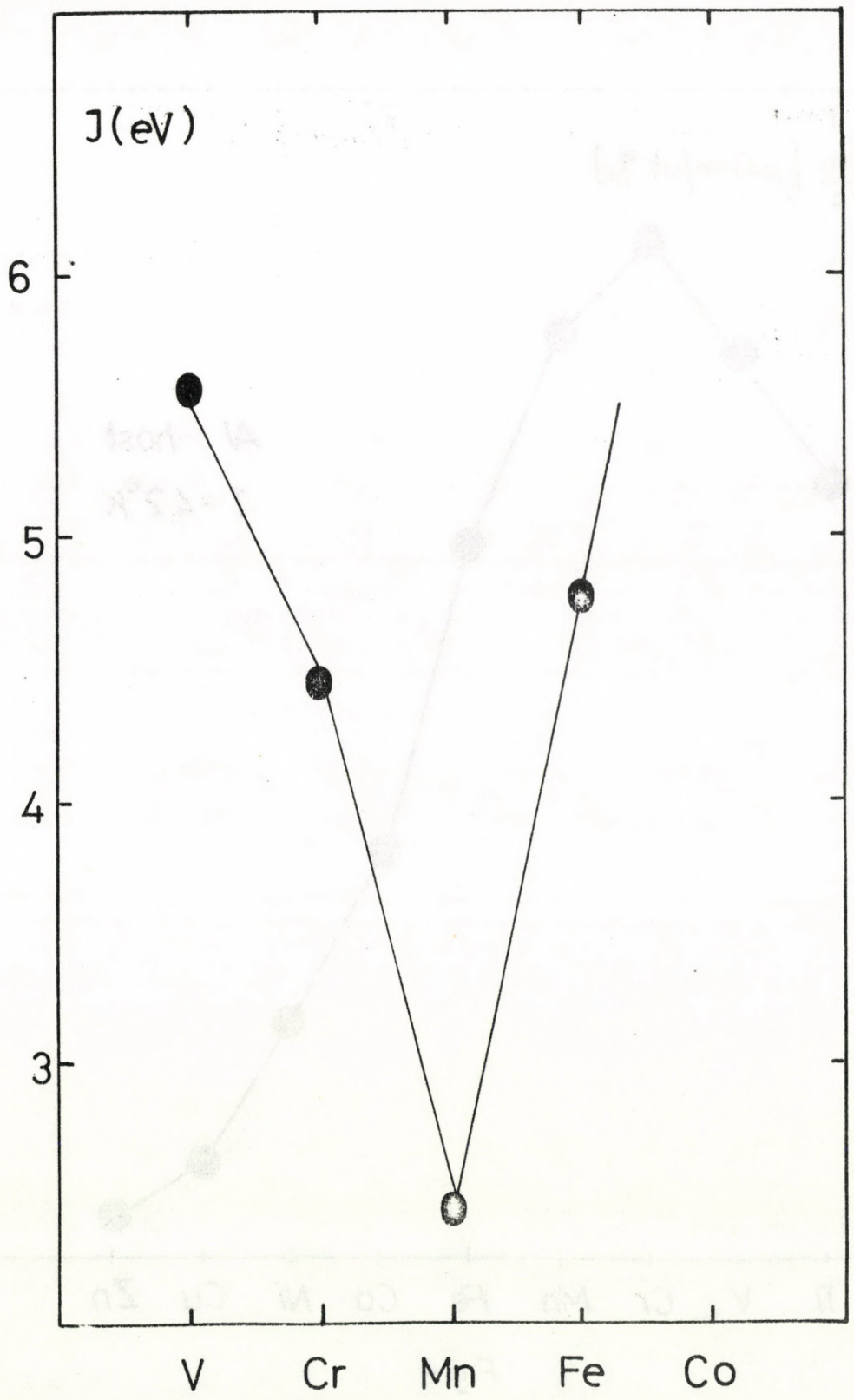


Fig. 5

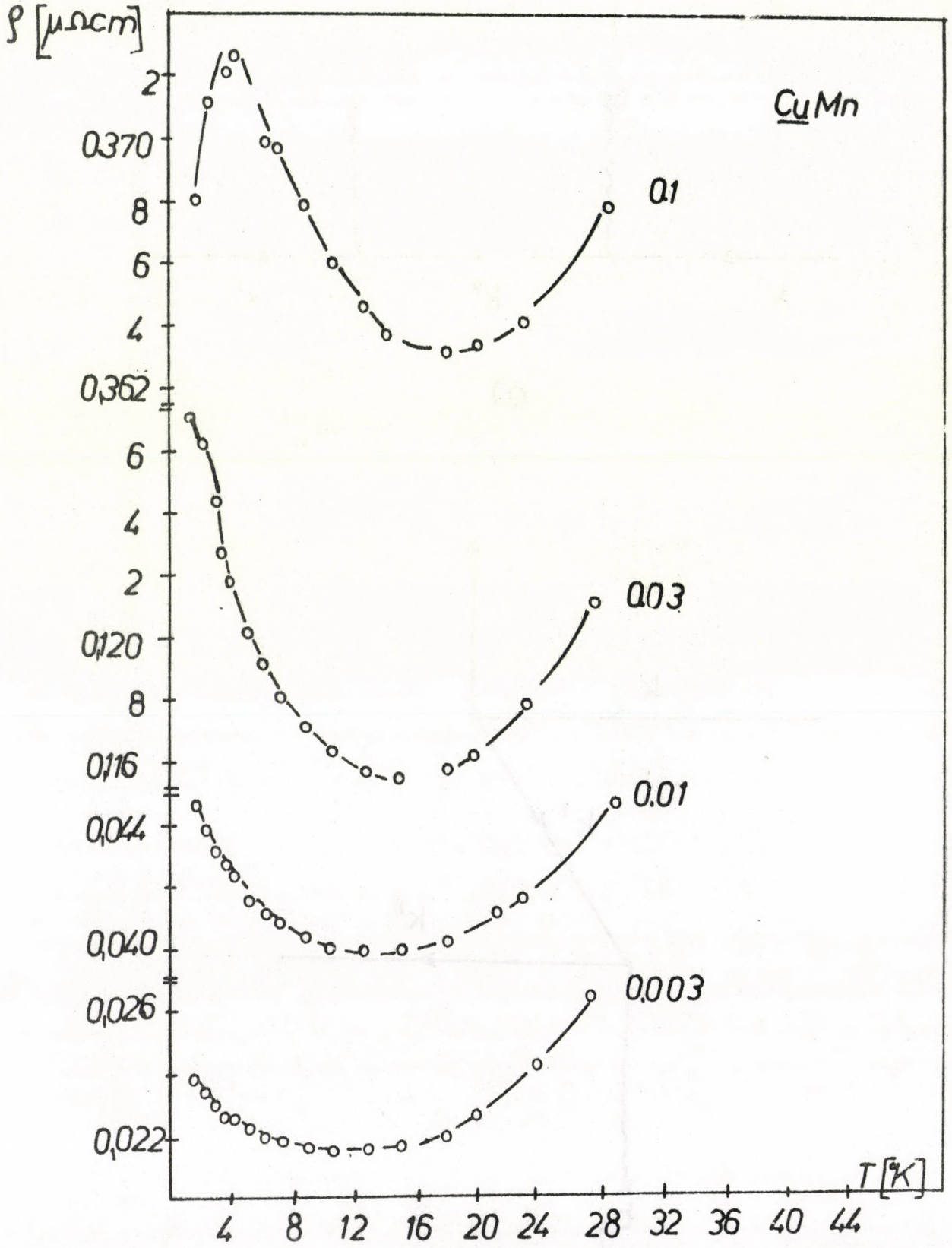
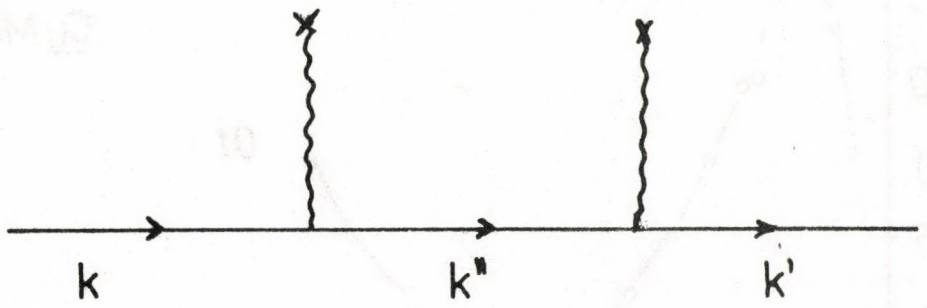
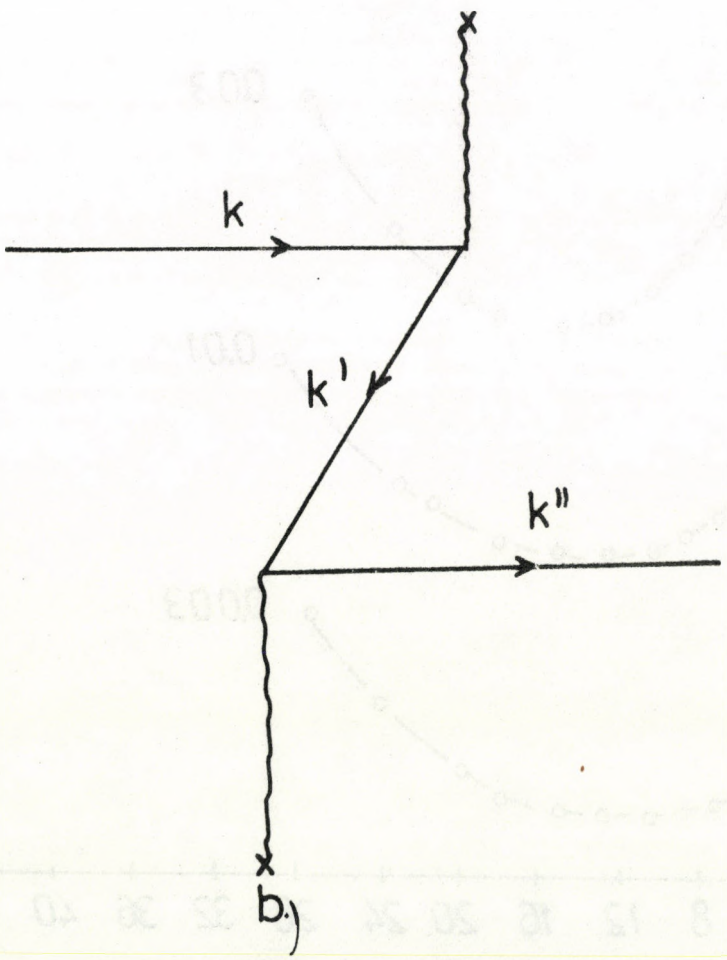

ρ [μΩcm]
CuMn
0.1
0.03
0.01
0.003
T [°K]
2
0,370
8
6
4
0,362
6
4
2
0,120
8
0,116
0,044
0,040
0,026
0,022
4
8
12
16
20
24
28
32
36
40
44

Fig.6



a.)



b.)

Fig. 7

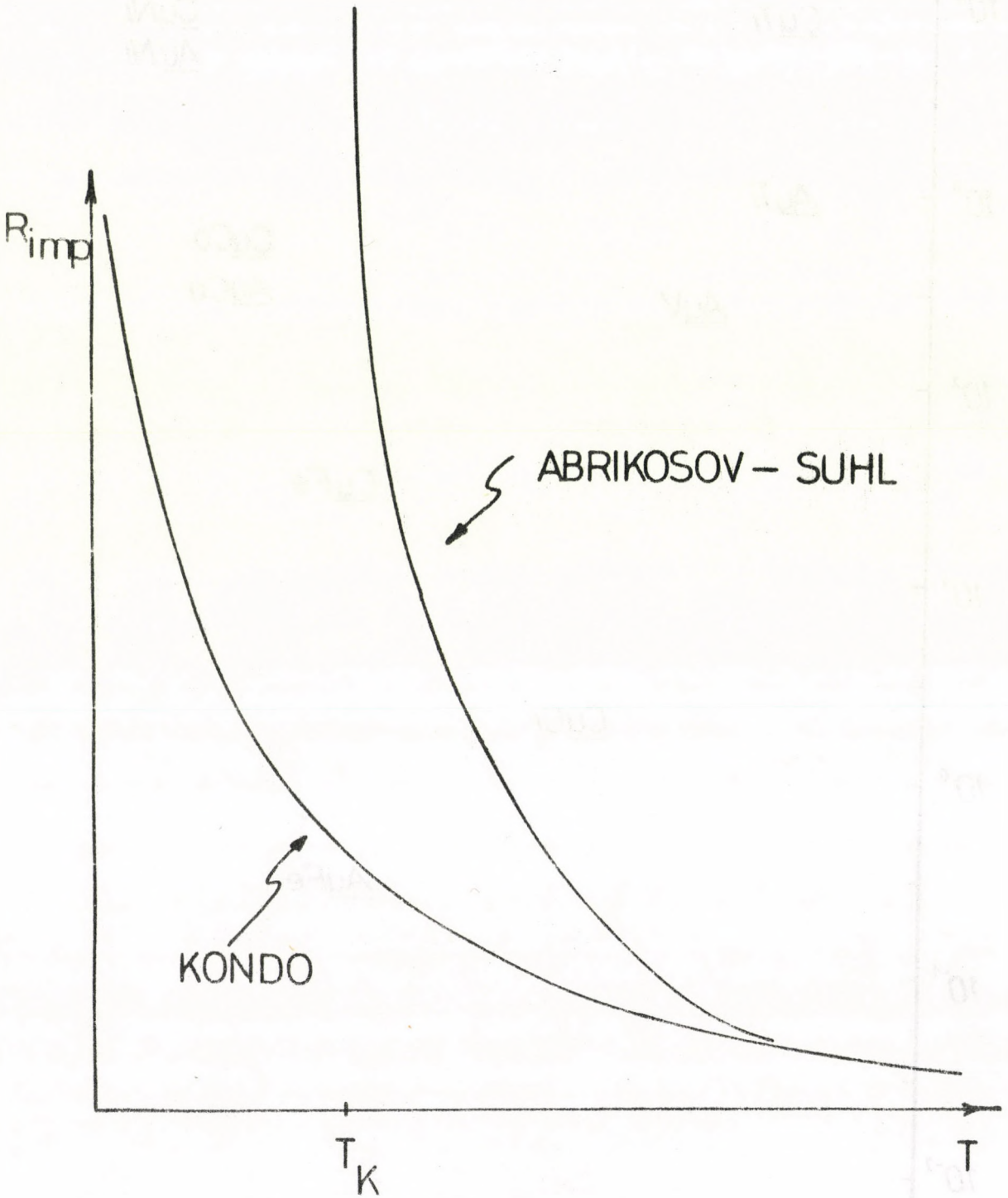
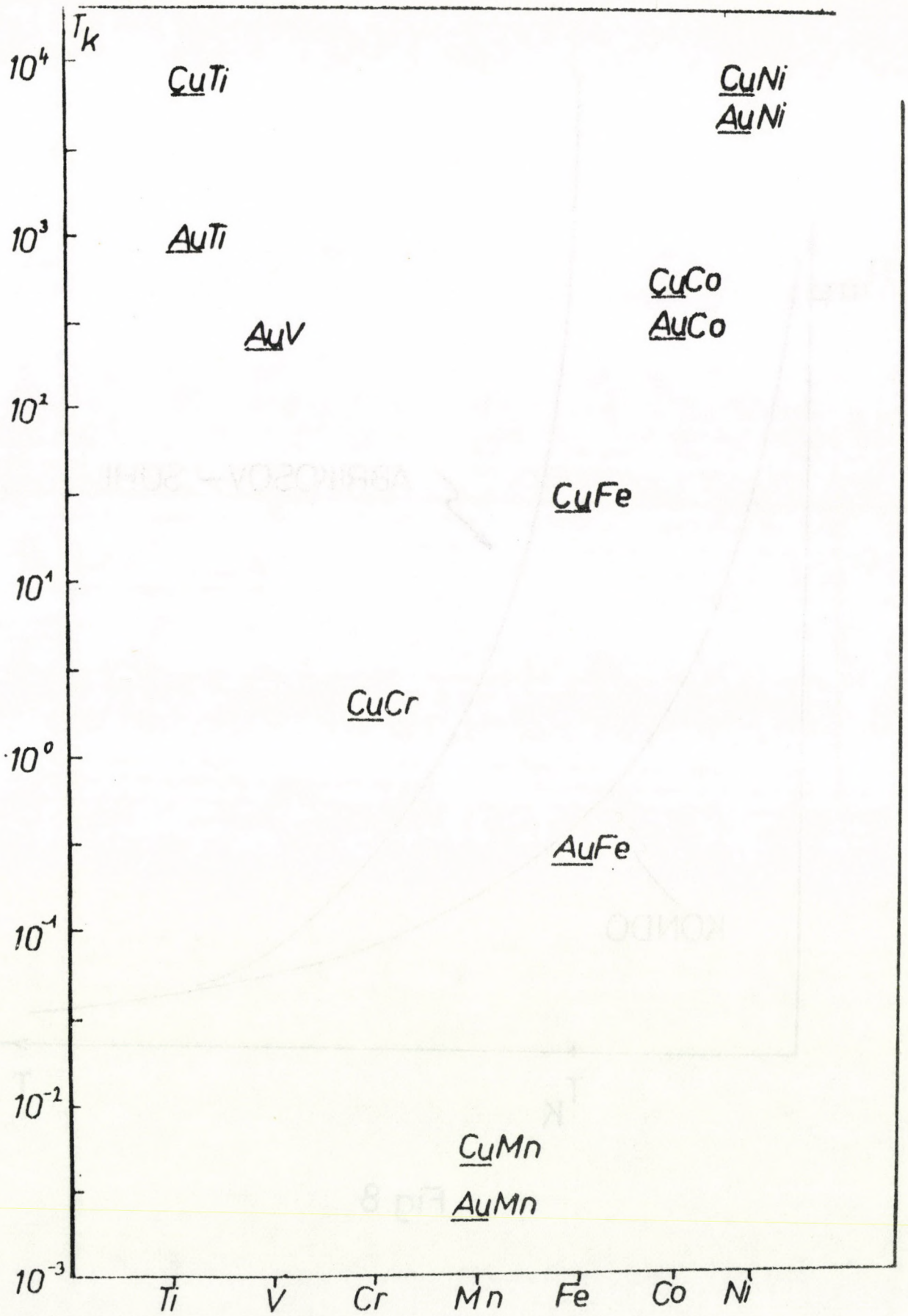


Fig. 8


T_K
10^4
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
CuTi
CuNi
AuNi
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CuCo
AuCo
AuV
CuFe
CuCr
AuFe
CuMn
AuMn
Ti
V
Cr
Mn
Fe
Co
Ni

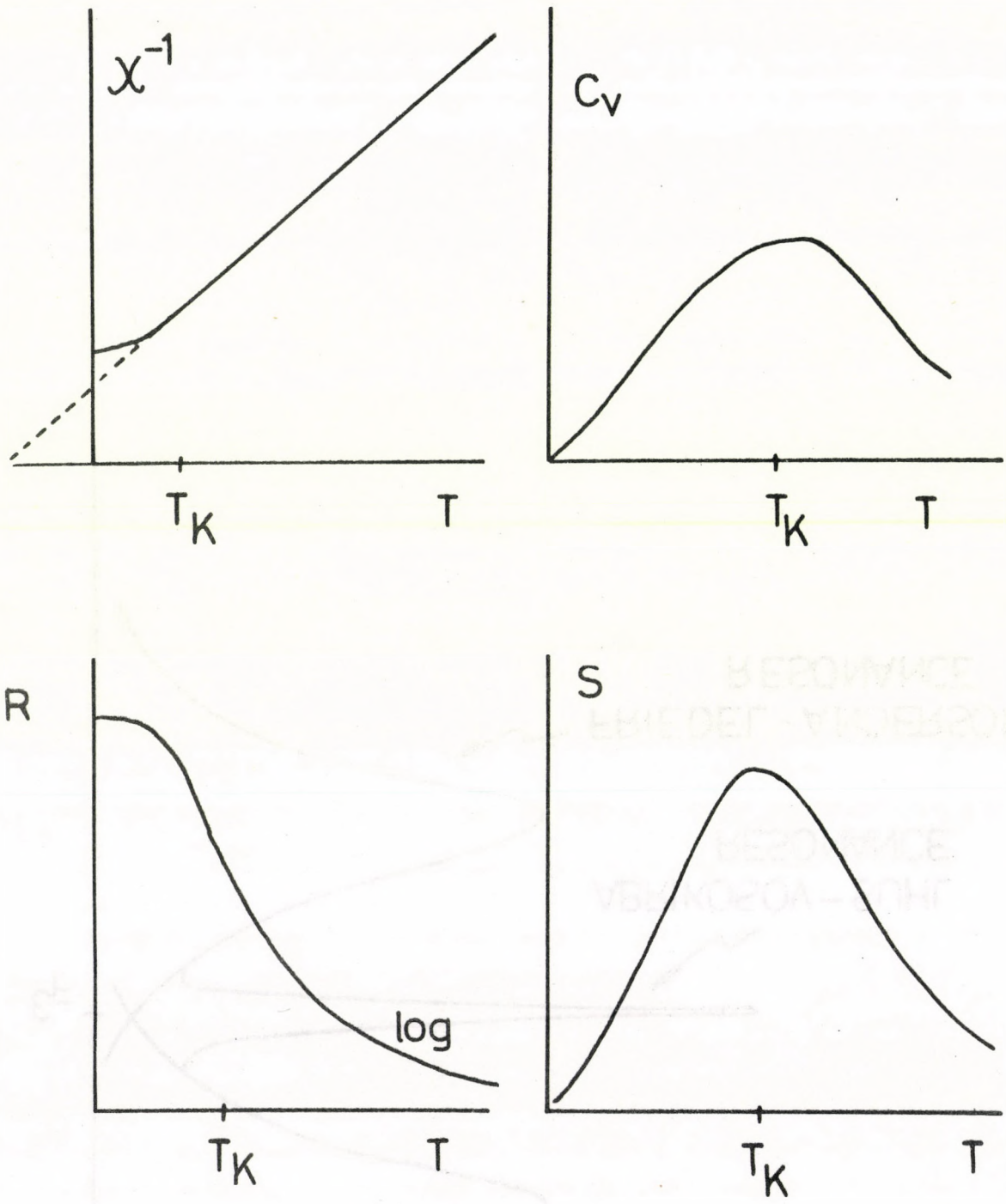
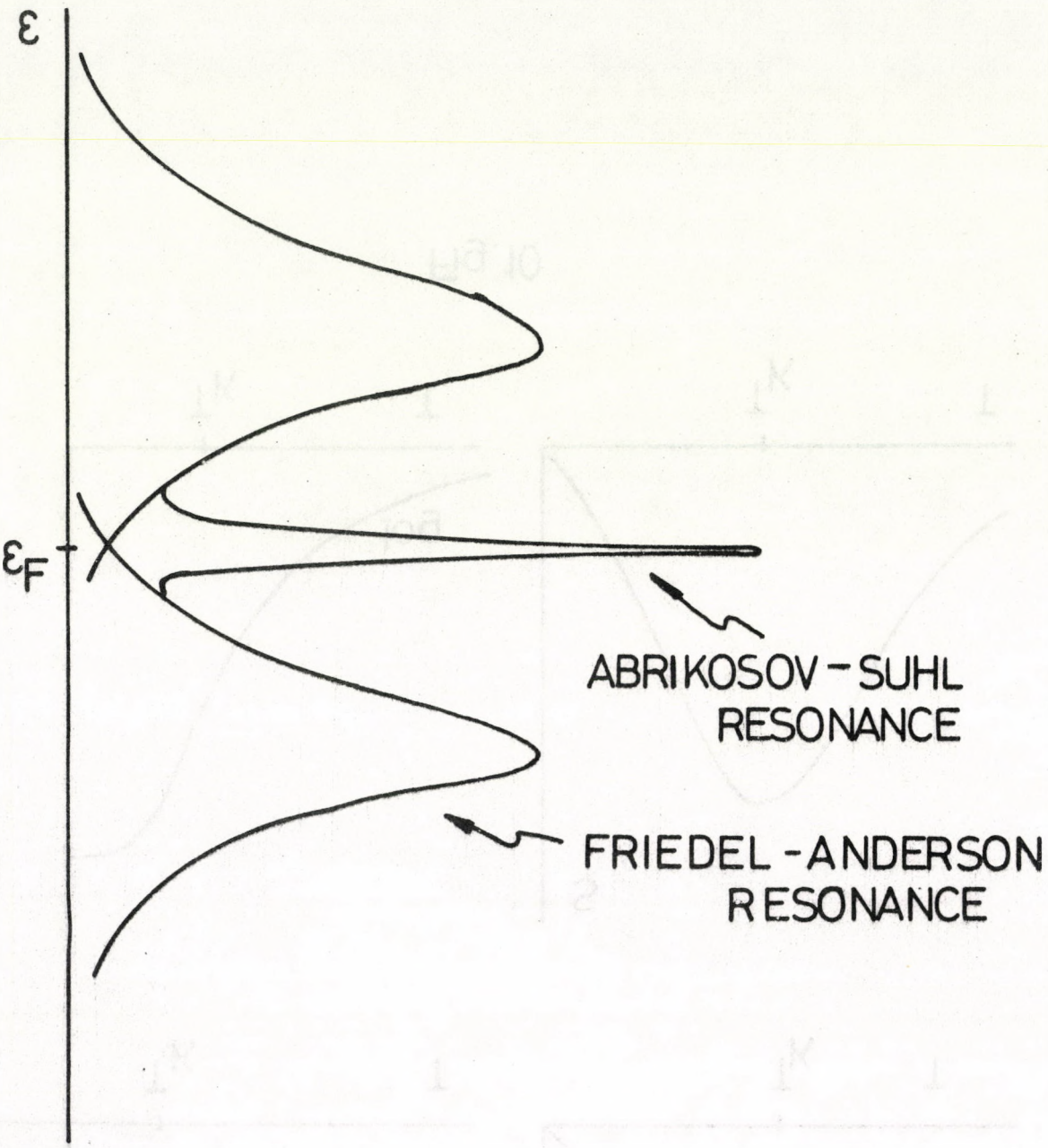


Fig.10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ε_F
ABRIKOSOV - SUHL
RESONANCE
FRIEDEL - ANDERSON
RESONANCE

Fig. 11

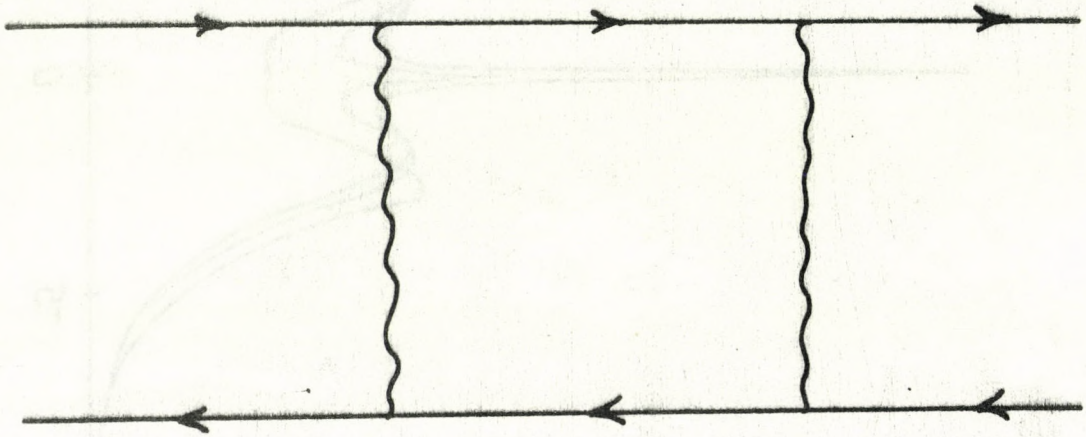


Fig. 12

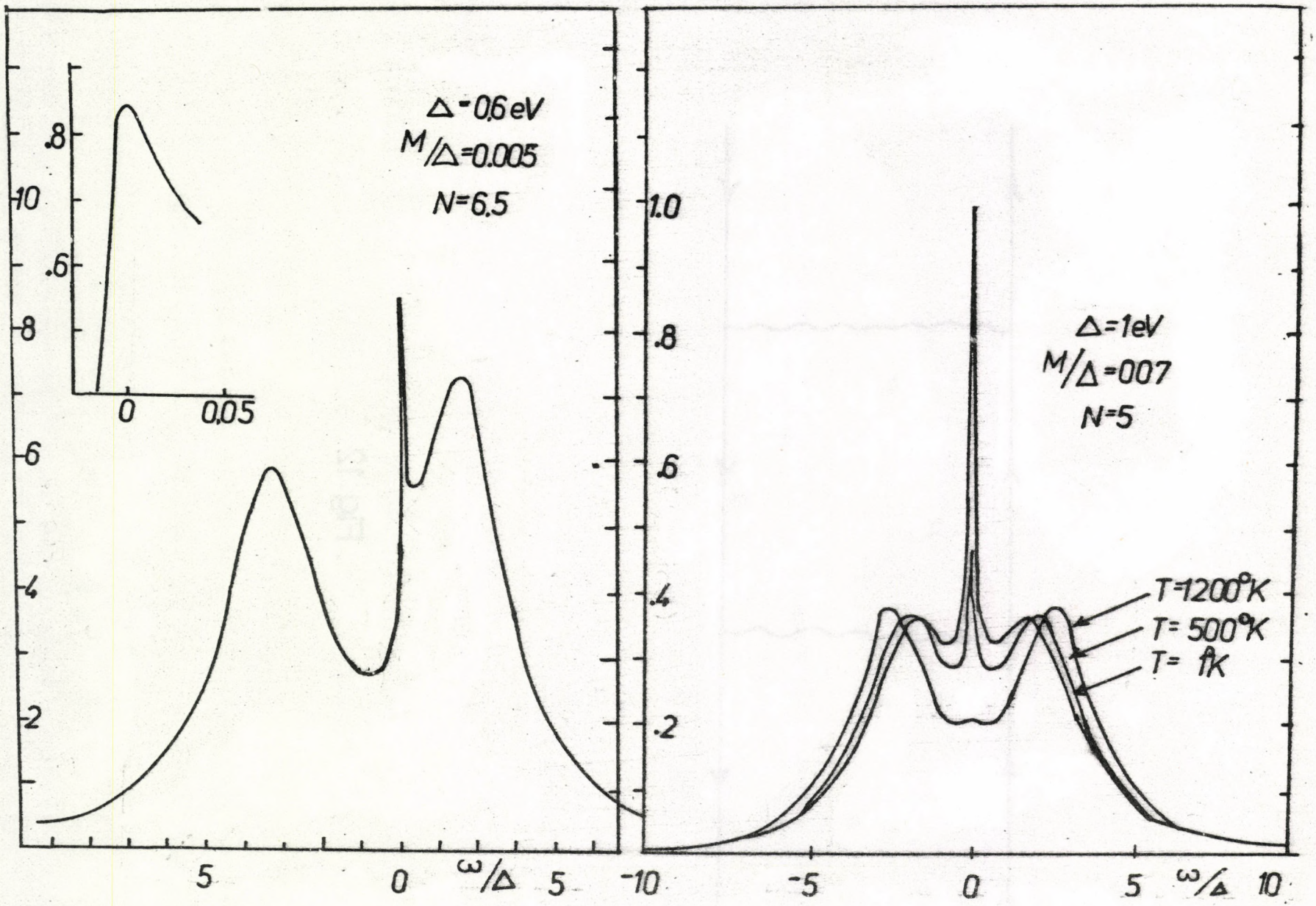
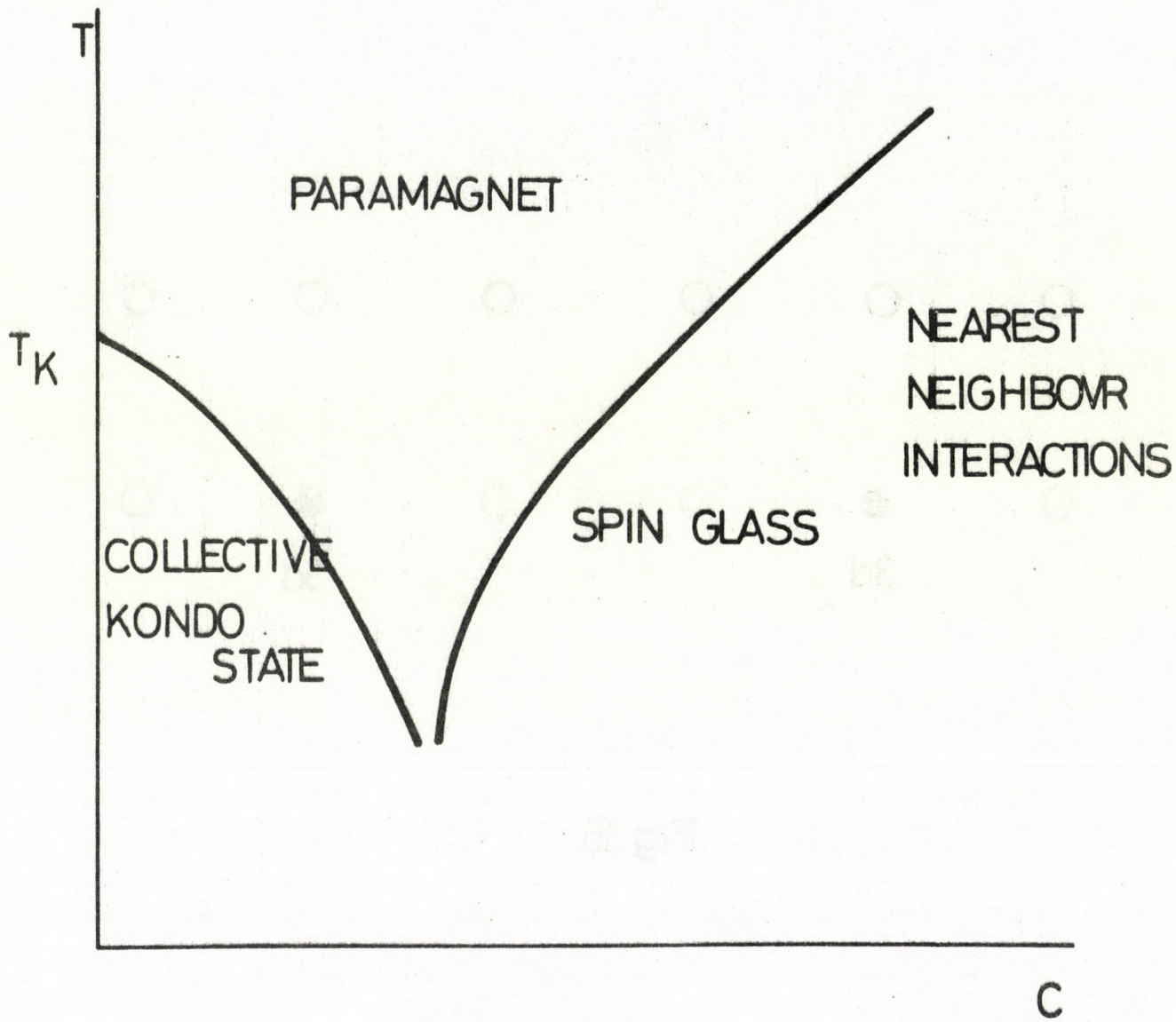


Fig. 13


T
PARAMAGNET
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C

Fig.14

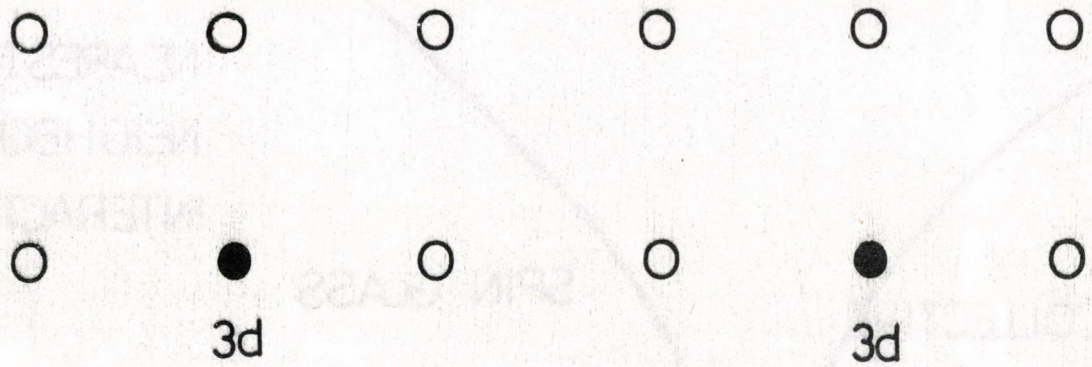


Fig.15

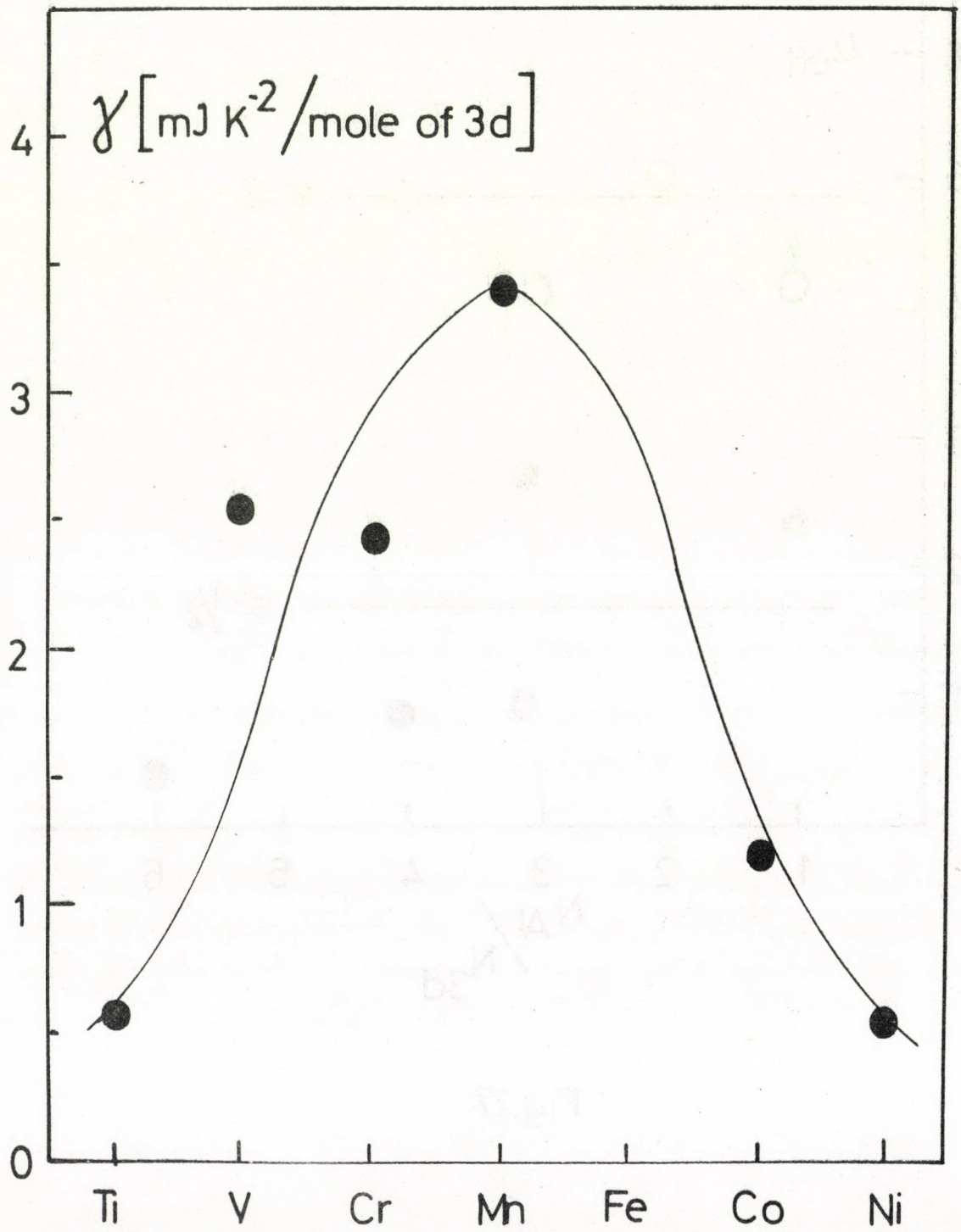


Fig. 16

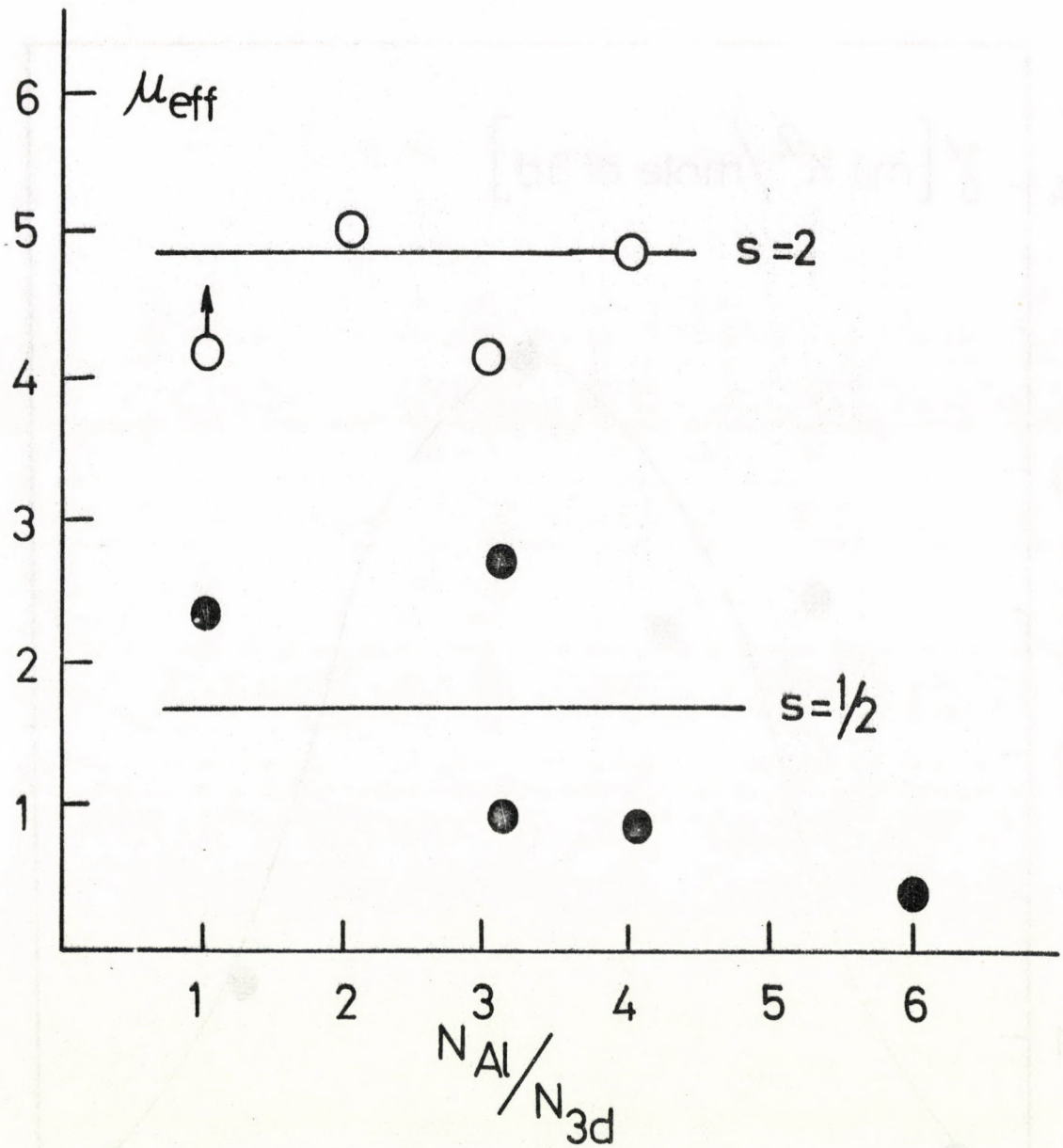


Fig.17

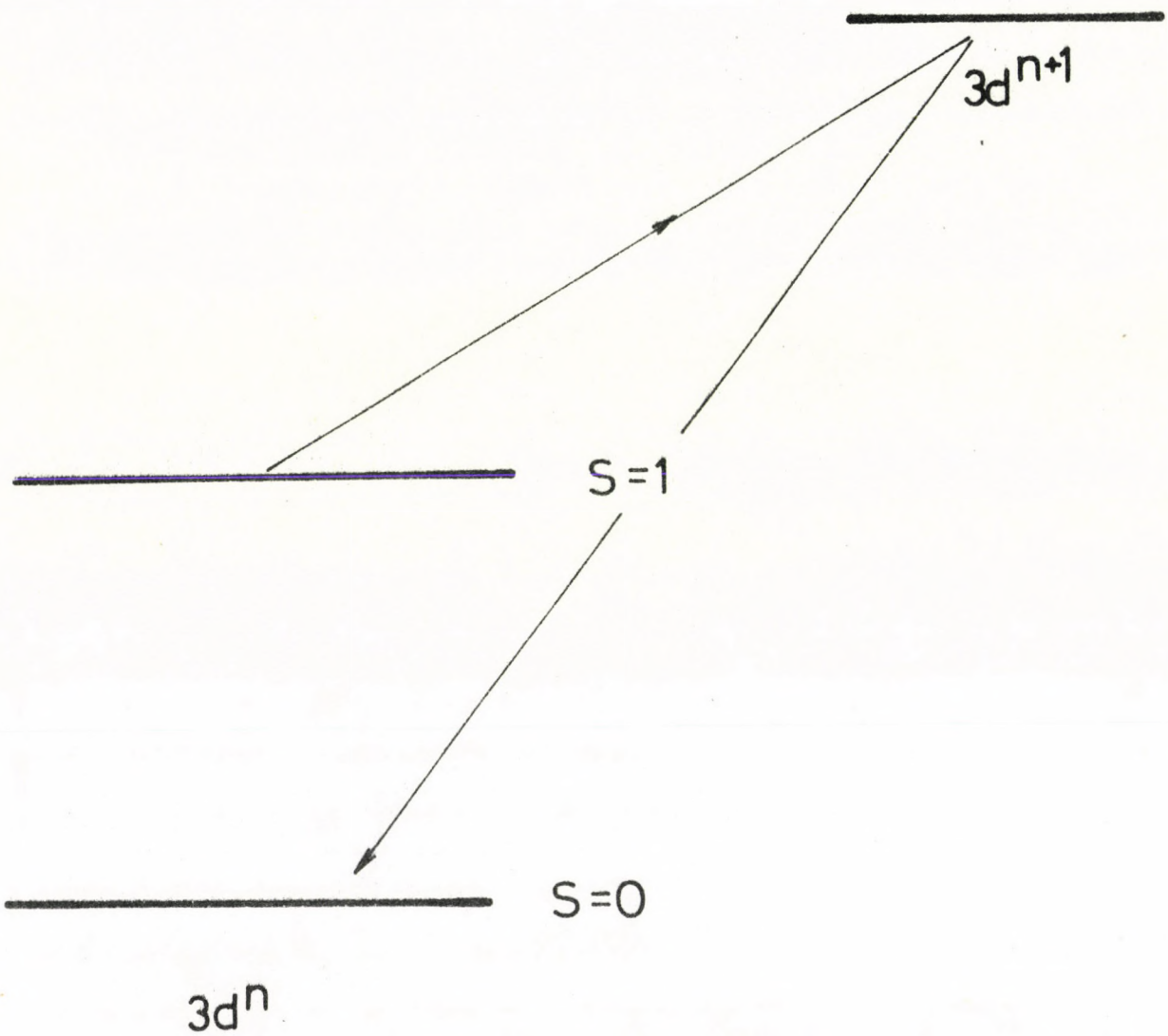
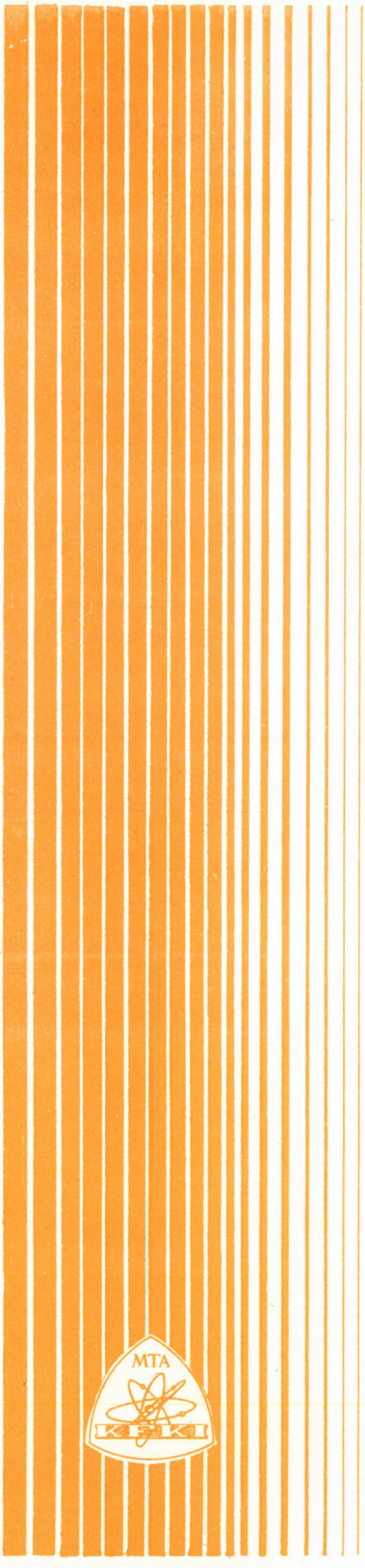


Fig. 18



Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Kósa Somogyi István
Szakmai lektor: Sólyom Jenő
Nyelvi lektor: Forgács Gábor
Példányszám: 65 Törzsszám: 76-988
Készült a KFKI sokszorosító üzemében
Budapest, 1976. október hó