PHYSICS OF HEAVY-FERMION SYSTEMS*

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A B S T R A C T

The understanding of conventional rare-earth intermetallic compounds is summarized by analysis of magnetic and electronic properties of conventional rare-earth intermetallic compounds. Conventional rare-earth compounds are understood well within the individualized-electron model in which *f* electrons are keeping their individuality also being part of the compound. In intermetallics there coexist itinerant/band electrons as well as localized *f* electrons which form a highly correlated electronic subsystem f^n. The analysis gives a clear evidence that the localized *f* electrons provide a substantial contribution to the specific heat, with the entropy of R ln2 in the case of Kramers ions. The *f* specific heat is extraordinarily large at lowest temperatures if the Kramers doublet ground state of the *f* subsystem is only slightly split. Such situation is supposed to occur in compounds exhibiting heavy-fermion phenomena. The heavy-fermion behavior is related to difficulties in the removal of the Kramers degeneracy of the f^n electronic subsystems that results in the small energy splitting δ. The removal of the Kramers degeneracy, that has to occur before the system reaches the absolute zero temperature, causes the appearance of two-closely-lying localized states with oppositely oriented local magnetic moments. Thermal excitations over the energy gap δ, that can be of order of 0.1 meV, cause the reversal of the local magnetic moment and subsequently pulls the reversal of the oscillatory spin polarization of conduction electrons. This complex object of the localized Kramers fermion with bounded conduction electrons can be regarded as a quasiparticle exhibiting bozonic properties. In this view, the heavy-fermion state is a magnetic, spin-wave state which is formed after breaking of the time-reversal symmetry. The splitting δ and the separation to the first excited CEF level Δ introduce two energy scales. Δ seems to be associated with the temperature denoted often as the Kondo temperature whereas δ - with the

width of the Kondo resonance thought to be at the Fermi level within the Fermi-liquid model. Two energy scales appeal from many experimental data.

The proposed model belongs to spin-transfer models. It is the first model that consistently explains low-temperature and high-temperature properties of heavy-fermion compounds independently on their metallic or ionic behavior. It is pointed out that localized *f* electrons do not contrast with the collective nature of the magnetic, heavy-fermion and superconducting states. In contrary to existing h-f theories the present theory reveals the microscopic origin of the phenomena. Due to this fact it has great prediction power. It offers, for instance, a novel look at the single-impurity Kondo problem. Namely, the formation of the weakly magnetic ground state of the magnetic impurity by the anisotropic charge distribution is argued to be superior to the original Kondo spin-compensation mechanism. It allows for the physical realization of the Kondo lattice understood at present as the collection of weakly-interacting paramagnetic ions with a small value of the local magnetic moment (small means a moment reduced by, say, 10 times compared with the free-ion value). Having this fact in mind, the present theory is not in conflict with many modern h-f theoretical approaches as the present theory discusses microscopic physical origin of the h-f phenomena in contrary to the other approaches that are largely phenomenological. The present approach reveals the physics of h-f particles and clearifies the problem of *f* states and *f* excitations. Distinguishing of these two notions removes the contradicted behaviour of *f* electrons. *f* electrons are in localized atomic-like states whereas their excitations can propagate through the lattice. The present theory fullfiles the basic requirement for the scientific theory: it can be experimentally verified and can be experimentally abolished.

Keywords: rare-earth compounds, heavy-fermion phenomena,
spin waves, Kramers degeneracy
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Glossary:

- a conventional rare-earth compound - a compound containing a rare-earth atom exhibiting properties well-understood, on the first glance, within the localized *f*-electron model,
- charge interactions - electrostatic interactions of the paramagnetic ion with surrounding charges,
- charge compensation mechanism - the formation of the weakly-magnetic state of a magnetic impurity in an metallic medium by electrostatic

interactions - it is caused by largely anisotropic charge distribution; compare with spin-compensation mechanism,
- heavy-fermion (h-f) phenomena - the most prominent is the large specific heat at low and ultra-low temperatures (below 1 K) that is not of nuclear origin; others are: a metallic behavior in magnetic fields characterized by almost temperature independent susceptibility that is taken as indication of a non-magnetic state and big changes in the temperature dependence of the resistivity, where a minimum can be found (with the temperature denoted as the Kondo temperature) and a low-temperature T^2 dependence.
- hybridization - it is widely used notion in physics and in chemistry for denoting the mixing of wave functions. In the h-f subject it is understood as the hybridization of *f* electrons with conduction electrons. Without clear specification the bare term hybridization is simply meaningless what happens quite often in literature.
- Kramers system - a f^n highly-correlated electron system of n *f* electrons, n is an odd number; also can be considered systems of d^n electrons and nuclear Kramers systems like ^{3}He.
- Kondo effect - the experimental effect of the increase of the resistivity with lowering temperature observed originally in diluted metallic system CuFe. The original paper by J. Kondo (Prog. Theor. Phys. **32** (1964) 37) has offered an explanation for this effect in terms of exchange interactions of the localized spin with spins of conduction electrons. It is proposed to keep the name of the Kondo effect for this experimental fact only.
- Kondo problem - a theoretical problem of the formation of the weakly-magnetic state of the magnetic impurity (single-impurity) that can be extended to the lattice of paramagnetic ions.
- Kondo spin-compensation mechanism - the formation of the nonmagnetic state of a magnetic impurity in an metallic medium by its cancellation by conduction electrons with opposite spins.
- Kondo-interaction mechanism - an interaction of the localized spin with conduction electrons described by the Kondo Hamiltonian.

Abbreviations: h-f - heavy fermion (state);
CEF - crystalline electric field; CF - charge formed (ground state);
S-D - spin dependent (interactions);
K-D -Kramers doublet; ELS -energy level scheme;
FES -fine electronic structure.
Energy units: 1 eV = 1000 meV, 1 meV = 11.6 K, 1 cm^{-1} = 1.44 K

From the author

It is not easy to write a book on the heavy-fermion systems. The heavy-fermion phenomena have been regarded by last 20 years, up to discovery of the high-T_c superconductivity, as the main problem of the modern magnetism. The difficulty is related with the fact that the subject is wide and exotic as well as that there is no consensus among the scientific community about the origin of these exotic phenomena despite of more than 20 years of extensive theoretical efforts.

Surely the author is taken the advantage of the fact that the h-f problem is not solved yet in order to propose a novel theory of heavy-fermion phenomena. The biggest point in favour of the present theory is that it is well founded in text-book magnetism and in metal physics and is based on general-symmetry considerations. The starting point of the theory is that the *f* electrons are taken to be localized in contrary to popular, at present, models based on delocalization of *f* electrons. But it is worth to point out that the localization of the *f* electrons and the starting single-ion point of view does not contrast with the collective nature of the magnetic and the superconducting state. Moreover, though the philosophy of the itinerant and localized-electron magnetism is basically different, in *f* intermetallics two electronic subsystems, described basically by these two different approaches, simply coexist. It is the beauty of the Nature to reconcile in this remarkable way this duality of the modern magnetism, is not it?

The novel way of understanding, as each novel way, comes to the scientific community with difficulties. Looking back to the history of Physics one finds that the most of new ideas came into Physics with troubles (e.g. black holes became accepted 50 years after its theoretical prediction). On this observation Karl Popper, a great philosopher of science, has formulated his theory about the revolutionary way of developing of Science. It is clear if one realizes that Physics is simply part of the human activity and due to this fact it subjects sociological rules. But fortunately, only partly and only for a limited time. In Science rules of the democracy do not work. In Science al-ways finally triumphs the objective scientific truth - one man over millions can be right providing a theory in agreement with the reality. Max Planck was likely right in his view about the mechanism for the spreading of new scientific ideas – new ideas win by dying of adherents of old ideas.

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I. Introduction

The role played by *f* electrons in rare-earth (4*f* metal) and uranium (one of 5*f* metals) intermetallic compounds is still very ambiguous. In so-called normal rare-earth compounds *f* electrons are found to be very well described within the localized-electron picture whereas in many compounds with Ce, Yb and mainly with uranium, known as heavy-fermion (h-f) compounds, the *f* electrons are believed to be highly delocalized, particularly at low temperatures [1-8]. The h-f compounds got so tremendous attention as this dual nature of the *f* electrons seems to appear in one compound as the function of temperature: *f* electrons exhibit the itinerant behavior at low temperatures and the localized behavior at high temperatures. Physical mechanism for this low-temperature delocalization is still under discussion [3,4,7], but the concept of delocalization of the *f* electrons plays the prominent role in the hybridization Fermi-liquid model and the Kondo-lattice model. These two models are nowadays two main theoretical approaches of the heavy-fermion phenomena. One should remember that these models deal with low-temperature h-f state and are not able to account for the crossover to the high-temperature localized-electron regime, for instance. A critical review of all existing models dealing with heavy-fermion phenomena has been recently given by Liu [7]. This review clearly shows that there is no consensus about the understanding of this hot topic in the modern magnetism. Such the situation calls for a new look and a new understanding. This paper offers a new understanding of the heavy-fermion problem [9,10].

The main borderline between models concerning heavy-fermion phenomena is associated with the role played by *f* electrons, namely if the *f* electrons are localized or delocalized. In conventional rare-earth compounds *f* electrons are found to be very well localized [11-14]. The hybridization model starts from the assumption that there is a strong hybridization of electronic states of *f* electrons and conduction electrons allowing for the hopping of *f* electrons to the conduction band and vice versa. It is further believed that the *f* electronic states lie close to the Fermi level, as an effect of the hybridization, and the local *f* moment is somehow dissolved by an admixture of *f* electrons with conduction electrons [6,8,11, for instance]. In a consequence one has a large specific heat at lowest temperatures and the Pauli-like enhanced susceptibility. The Fermi-liquid model deals with properties of the h-f state but does not have any hint to explain the smooth transformation with increase

of temperature of the h-f state to the opposite limit, i.e. the localized-moment state. It is highly intriguing how the increase of temperature sometimes by 10-20 K, which corresponds to the energy of about 0.002 eV, can drive the shift of the *f* electronic states down by 2-5 eV. In Kondo-type explanations for the formation of the non-magnetic state, it is assumed that below a certain temperature a bound state of the (significant) localized spin/moment and conduction electrons is formed, in which the (significant) local moment of the magnetic impurity is fully compensated by antiparallelly oriented spins of conduction electrons (this mechanism will be called for better clearity as the Kondo spin-compensation mechanism for the formation of the nonmagnetic state of magnetic impurity). This single-impurity Kondo model extended to the Kondo lattice, however, meets serious objections. Noziéres has pointed out that in the Kondo lattice there is not sufficient number of conduction electrons to compensate all localized moment by means of the spin-compensation mechanism [15]. One tries to remove this objection by considering the Kondo particle as composed from two *f* ions being strongly antiferromagnetically coupled. Such picture is, however, not confirmed experimentally. In this point it is necessary to worn about misleading word-proximity of the Kondo-lattice model and the single-impurity Kondo-model. Unfortunately, the Kondo-lattice model has little in common with the single-impurity Kondo model. The single-impurity Kondo model considers a localized state having a spin-degree of freedom interacting with conduction electrons purely via spins. In the Kondo-lattice model the charge transfer processes are playing essential role in formation of the heavy-fermion state.

The Kondo lattice is not the lattice of Kondo single-impurities. One can formulate the key h-f problem of localization or delocalization of *f* electrons by considering how in a dense system the *f* electrons may communicate with each other. In hybridization Fermi-liquid model or the Kondo-lattice model communication goes via intersite electron hopping (the charge transfer). The presented model employs communications via spins and is a spin-transfer model. The interaction of two localized spins via conduction electrons is known as the RKKY interaction. Then one can considers the RKKY interaction as somehow the double single-impurity Kondo interactions.

In this paper, the understanding of conventional rare-earth intermetallics, in which *f* electrons are treated as fully localized, is summarized. Within these concepts the understanding of the h-f phenomena is proposed. It turns out that, the h-f phenomena can occur for Kramers systems and the h-f behavior is related with difficulties in the removal of the Kramers degeneracy at low

temperatures. In order to avoid possible misunderstandings it is worth to mention that the localized *f* electrons do not contrast with the collective nature of magnetic and superconducting phenomena. The paper is organized as follows: at first, the understanding of conventional rare-earth is summarized, that allows for the presentation of the individualized-electron model. Latter, the novel understanding of heavy-fermion phenomena within the CEF and Kondo-effect model is presented together with some consequences and predictions of the model.

II. The understanding of *f* intermetallics - a short overview

Electronic and magnetic properties of normal rare-earth intermetallics, like $NdNi_5$ or $ErNi_5$, are well understood by considering the electronic system of an intermetallic compound as composed from a few electronic subsystems. It is essential to distinguish the *f* electronic subsystem from the conduction-electron (c-e) subsystem. The c-e subsystem is of the single-electron nature and shows in intermetallics rather simple behavior. In RNi_5 compounds, for instance, it is described [11-14] by a value for the Sommerfeld coefficient γ^c of 36 mJ/K^2 mol f.u. and the susceptibility χ^c of $4*10^{-3}$ μ_B/T f.u. (^{c} - denotes the c-e subsystem). The *f* electronic subsystem is a many - electron subsystem f^n in which spin and orbital movements of n electrons are highly correlated (by the Coulomb interactions and spin-orbit interactions). The many-electron states form, much below the Fermi level, a discrete energy spectrum, called fine electronic structure (FES) due to its strict analogy to the fine structure occurring in the atomic physics. E_F is placed in the c-e band and is associated with single-electron excitations. Properties of the *f* subsystem, like the specific heat, the ordered magnetic moment or the paramagnetic susceptibility and its anisotropy, are understood within the localized-electron magnetism. Referring to two limits, known as the localized-electron model and the band/itinerant-electron model, this approach to *f* intermetallics one can call as an individualized-electron model [now we called it as the Quantum Atomistic Solid-State Theory QUASST]. It underlines the fact that different electronic subsystems, described in the localized-electron and band-electron model, coexist in one *f* intermetallic compound. Moreover, this name underlines the fact that *f* electrons, of different atoms constituting the intermetallic compound, remember also in the solid their atomic individuality. This individualized-electron model successfully describes properties of conventional rare-earth intermetallics [14].

An important outcome from different experiments is that in most of the

compounds containing rare-earth ions, the *f* electrons are giving dominant contribution to electronic and magnetic properties. This is illustrated in Fig. 1 where properties of $ErNi_5$ and $LaNi_5$ are compared.

Primary interactions between the *f*-shell electronic subsystems and the conduction-electron subsystem are direct electrostatic interactions. Apart of these direct charge interactions there are also spin-dependent (S-D) interactions which are usually much weaker. These S-D interactions mainly manifest at low temperatures being the origin of the appearance of the magnetic state. These two interactions refer to Stark and Zeeman effects, respectively, in the text-books dealing with atomic physics. The S-D interactions commonly named exchange interactions though no direct exchange of electrons is necessary for their occurrence [16]. Owing to the large interatomic R-R distance the S-D interactions between *f* electrons are mediated by conduction electrons as is discussed in the RKKY interactions. Among conduction electrons, Campbell [17] has emphasized the role played by own 5*d* electrons. The scheme for two *f*-spins interacting via own 5*d* spins has been shown in [18].

The *f* subsystem is a highly correlated f^n electronic system, in which the spin and orbital movements of n *f* electrons are highly correlated implying that the total angular momentum **J** serves as the good quantum number. There is also a very strong correlation between the charge distribution around the *f*-shell electrons, largely determined by conduction electrons, and the magnetic characteristics of the ground state of the *f* electronic subsystem. This effect leads to a suppression of the local magnetic moment. In some cases it can lead to a fully non-magnetic ground state. It has been well-known for non-Kramers systems. Such possibility for a Kramers system has been for the first time proved by Radwanski [19]. This theoretical proof is of great importance in case of Kramers systems. This effect, known as the charge-formation of the non-magnetic (weakly-magnetic) ground state of the magnetic impurity, is an alternative mechanism to the Kondo spin-formation mechanism [20]. Moreover, it has been argued that this charge mechanism is much more effective compared with the spin mechanism.

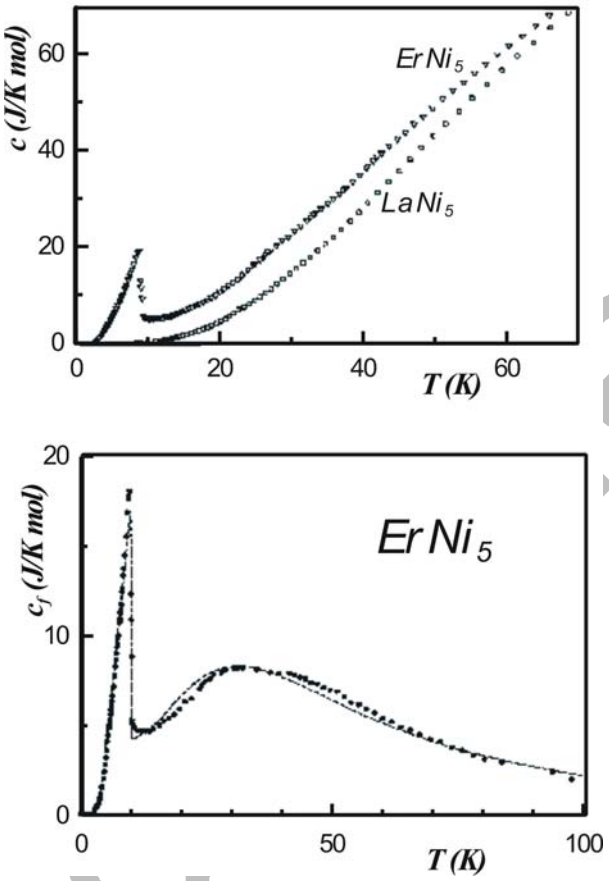

Fig. 1. a) Temperature variation of the specific heat of $ErNi_5$ and $LaNi_5$.

b) The excess of the specific heat of $ErNi_5$ compared with $LaNi_5$ is attributed to the *f* electronic subsystem and is associated with many-electron excitations over the localized states of the f^{11} electronic subsystem. The λ-type of peak is associated with the occurrence of the long-range magnetic order; its position at T_c of 9 K is determined by the exchange interactions between the Er spins. The conduction-electron specific heat in $LaNi_5$, that is a straight line with the coefficient γ^c of 36 mJ/K^2 mol f.u. is only a small part of the specific heat associated with the *f* electrons except the lowest temperatures. After ref. 11.

An *f* paramagnetic ion, when placed in a solid, experiences the electric-field potential due to all charges constituting the solid. As an effect of this potential, the orbital degeneracy of the partially filled *f* shell is lifted and different charge-formed (CF) ground states of the *f* subsystem are realized. In Fig. 2, the energy level scheme (ELS) for the Er^{+} ion in $ErNi_5$ is shown [12] that has been derived by careful and combined analysis of all known experimental data including temperature dependence of the specific heat, magnetization curves up to 35 T on single crystalline specimen and inelastic-neutron scattering experiments. The good fit indicates that the CEF levels are really thin, with a width below 0.2 K. The Er^{3+} ion is the f^{11} Kramers system with L=6, S=3/2 J=15/2 and g=6/5. In fig. 3 the temperature dependence of the specific heat of $NdNi_5$ is shown in comparison to that of YNi_5. In Fig. 4 the energy level scheme of the Nd^{3+} ion in $NdNi_5$ under the CEF interactions of the hexagonal symmetry is shown [21,22]. The Nd^{3+} ion in $NdNi_5$ is a f^{3} subsystem (the system with 3 *f* electrons). This ELS is relevant also for the Pr^{2+}, Nd^{3+}, U^{3+} or Np^{4+} ion. This energy level scheme contains five doublet Kramers states as the f^3 system, being a Kramers system, is characterized by the total angular momentum J of 9/2. The shown states belong to the ground multiplet $^4I_{9/2}$. The excited multiplet lies 270 meV above. Thus the overall CEF splitting amounts to 8% of the separation to the first excited multiplet. It results from the fact that spin-orbit interactions are much stronger than CEF interactions what is general rule for *f* ions. In case of $NdNi_5$ the splitting of the Kramers-doublet ground state below T_c of 7 K, due to the appearance of the internal magnetic field, amounts to 7.9 K at 0 K [23,24]. This splitting is a source of the great number of excitations observed in specific-heat experiments at temperatures comparable to the energy splitting. **In specific-heat experiments**, even at lowest temperatures, many-electron excitations of the *f* subsystem over the energy level scheme are superimposed on single-electron excitations, at the Fermi level, associated with conduction electrons. It is in the similar way as excitations over the nuclear states are superimposed in ultra-lowest temperatures though the nuclear states are certainly not lying at the Fermi level. Nuclear excitations in Ho_2Co_{17}, for instance, are observable in specific heat experiments already at 3 K [25]. For the reason of description it is useful to introduce apart of the Fermi level the excitation level, Fig. 5, that passes through the Fermi level, the *f* ground state and the nuclear ground state.

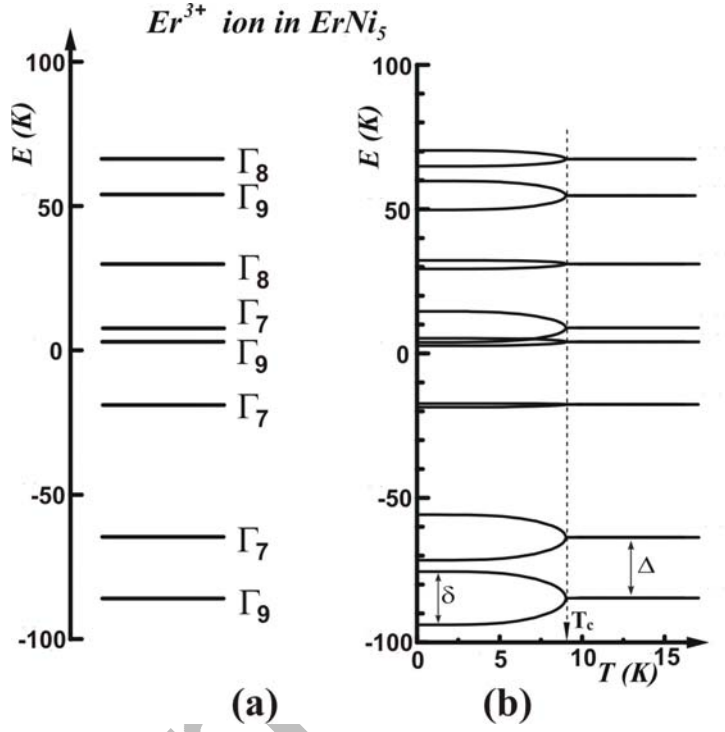

Fig. 2. a) the charge-formed localized states of the f^{11} Kramers system of the Er^{3+} ion in $ErNi_5$.

b) Effect of the exchange interactions on the many-electron states of the Er^{3+} ion in $ErNi_5$. The Kramers doublets are split in the magnetically ordered state i.e. below T_c. The collapsing of the ground state Kramers doublet gives a λ-type peak at vicinity of T_c with the entropy equal to Rln2. δ and Δ denote the splitting of the Kramers-doublet ground state and the separation to the first excited CEF level. These states are many-electron bound states existing 6 eV below the Fermi level. The population of these states is governed by the Boltzmann-distribution function - at the absolute zero temperature only the lowest state is occupied. With increasing temperature higher states become occupied resulting in given temperature dependence of the specific heat, of the magnetic moment, of the magnetic susceptibility and other properties. After Ref. [12].

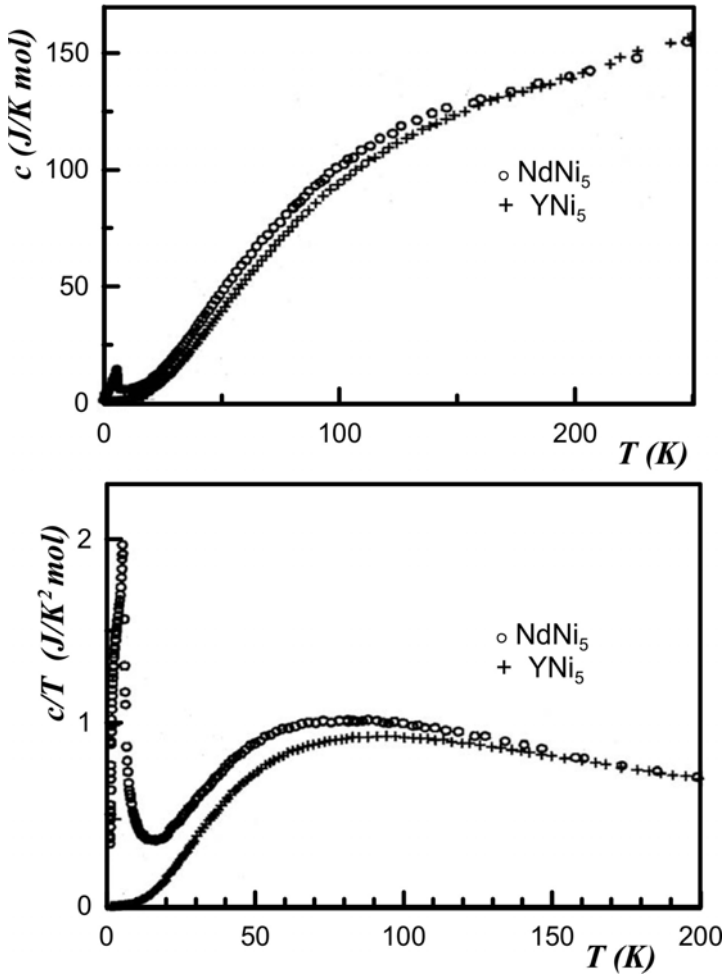

Fig. 3. Temperature variation of the specific heat of $NdNi_5$ together with the specific heat of YNi_5. The excess of the specific heat in $NdNi_5$ is attributed to the *f* electronic subsystem and is associated with many-electron excitations over the localized states of the f^3 electronic subsystem. The λ-type of peak is associated with the occurrence of the long-range magnetic order; its position at T_c of 7 K is determined by the exchange interactions between the Nd spins. Taken after ref. 21.

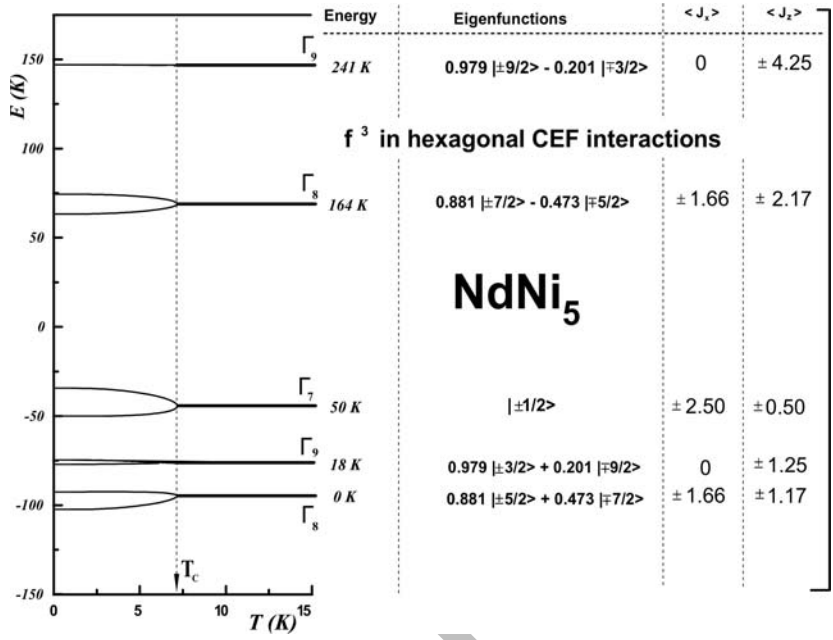

Fig. 4. The energy level scheme for the Nd^{3+} ion in $NdNi_5$ under CEF interactions of hexagonal symmetry together with the eigenfuctions and the expected values for $<J_x>$ and $<J_z>$. All levels are Kramers doublets and they are split in the magnetically-ordered state below T_c of 7 K where $NdNi_5$ becomes ferromagnetic. The CEF parameters are $B_2^0 = +3.35$ K, $B_4^0 = +14.5$ mK, $B_6^0 = -0.35$ mK, $B_6^6 = -13.5$ mK and the molecular-field coefficient between the Nd moments amounts to 3.5 T f.u./μ_B. After Refs [22,23].

A substantial reduction of the local magnetic moment is another important point. In $NdNi_5$, for instance, the ordered moment at 1.5 K amounts to 2.1 μ_B. It is roughly half of the full trivalent Nd moment of 3.27 μ_B which is found in the absence of CEF interactions. It is manifestation of the suppression of the local magnetic moment by anisotropic charge (electrostatic) interactions. In Ref. [19] I have proved that the anisotropic charge interactions can fully suppress the local moment even in case of the the Kramers systems indicating that the charge interactions can form any value of the local magnetic moment, between zero and the maximal value of $g\mu_B J$. Secondly, it means that not

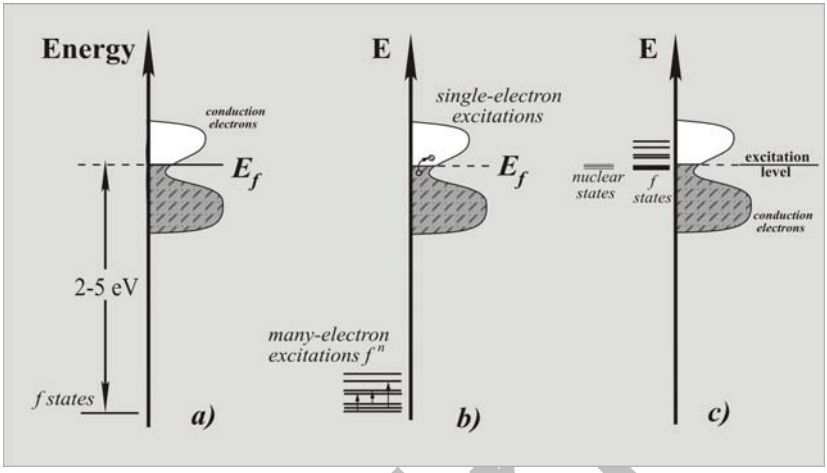

Fig. 5. The Fermi level and the excitation level in *f* intermetallic compounds. The Fermi level as associated with single-electron excitations lies in the conduction band. The *f* localized states lie 2-5 eV below the Fermi level though excitations of the f^n system can have very small energy being detectable at low temperatures. Also nuclear excitations can be observed at low temperatures though the nuclear states are lying a few GeV below E_F. The excitation level passes through the Fermi level, the *f* ground state and the nuclear ground state.

always the Kramers doublet can be represented by effective spin 1/2, i.e. that the action of external field is not always linear with the field.

In a summary, studies of conventional rare-earth compounds obviously show that magnetic, electronic and transport properties of an intermetallic compound critically depend on details of the fine electronic structure of the f^n subsystem, i.e. on the energy separations and the shape of the *f* ground state. The knowledge of the shape of the *f* ground state like magnetic characteristics is decisive for analysis of properties at temperature region below 5 K. This studies clearly show that the description of the doublet by an effective spin S=1/2 is not able to reflect the wealth of the phenomena produced in reality by the Kramers doublet ground state in different lattices. The existence of this fine structure indicates that *f*-band models treating the *f* band as the S=1/2 uniform has to be improved. An important point is that the *f* localized

electrons are the source of the magnetism in the system, in particular in case of the Kramers system. It justifies the starting point of the presented approach into the collective h-f state from the *f* electronic system(s).

This approach has been applied to some 5*f* compounds like UGa_2 and UPd_2Al_3. UPd_2Al_3 is an antiferromagnetic superconductor. Its overall temperature dependence of the specific heat, the value of T_N (14 K) and the magnetic moment have been well described within this approach assuming the U^{3+} ($5f^3$) configuration with B_2^0= +7.5K, B_4^0=+60 mK, B_6^0= +0.07 mK and B_6^6= -32 mK [26,27]. UGa_2 is ferromagnet with T_c of 125 K and the ordered

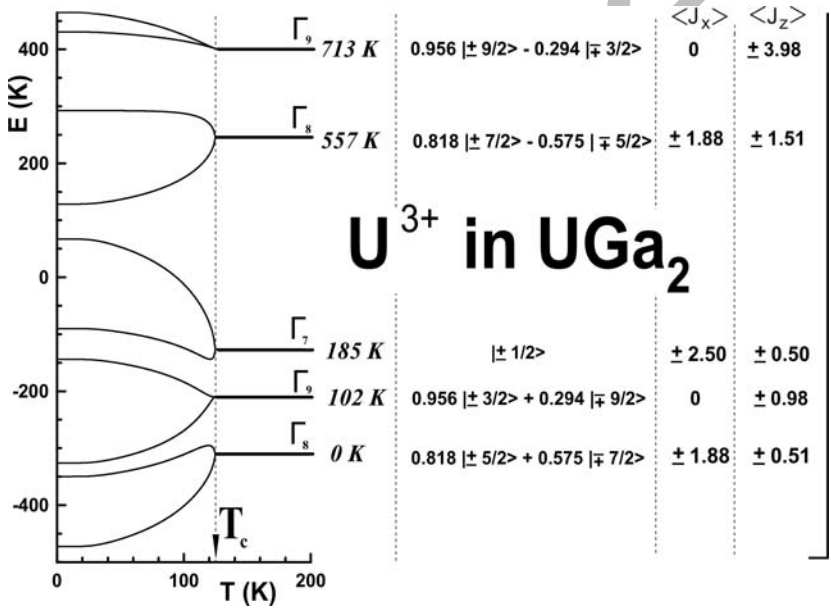

Fig. 6. The energy level scheme for the U^{3+} ion in UGa_2 under CEF interactions of hexagonal symmetry together with the eigenfuctions and the expected values for $\langle J_x \rangle$ and $\langle J_z \rangle$. All levels are Kramers doublets and they are split in the ordered state below T_c of 125 K where UGa_2 becomes ferromagnetic. The CEF parameters are B_2^0 = + 8.38 K, B_4^0= + 36.25 mK, B_6^0= -0.5 mK, B_6^6 = -52 mK and the molecular-field coefficient between the Nd moments amounts to 40 T f.u./μ_B. After ref. 24.

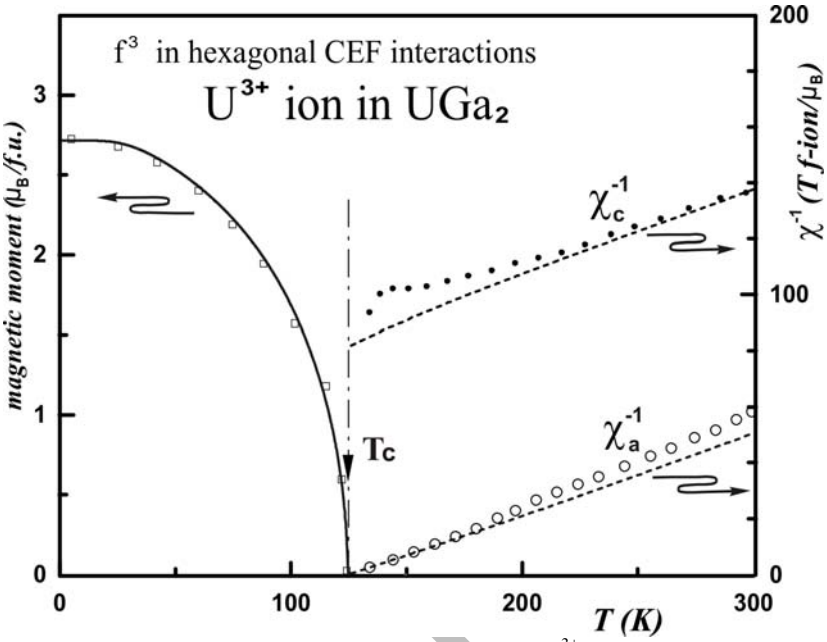

Fig. 7. The calculated temperature variation of the U^{3+} magnetic moment (left scale) and of the reciprocal susceptibility (right scale) resulting from the CEF parameters listed in Table 1. Points are data measured for the monocrystalline UGa_2. After Ref. [24].

moment of 2.7 μ_B. Its magnetic and electronic properties have been well described assuming again the U^{3+} ($5f^3$) configuration with B_2^0= +8.38K, B_4^0=+36.25 mK, B_6^0= -0.5 mK and B_6^6= -52 mK [24]. The derived energy level scheme is shown in Fig. 6. Good reproduction of experimental results, like specific heat and the value of the ordered local moment as well as of the value of T_c, provides strong argument for the existence of the localized *f* electrons also in (some) uranium intermetallics. Surely it will be of great interest to check how far this applicability goes in other compounds. The temperature dependence of the localized levels in the ordered state in UGa_2 is much more complex compared with $NdNi_5$ due to much stronger S-D interactions. The Curie temperature of UGa_2 is almost 15 times bigger than $NdNi_5$.

In Fig. 7 the temperature dependence of the local magnetic moment in the ordered state in UGa_2 is compared with experimental data as well as of the

susceptibility measured on the single-crystal specimen [24]. One can see that the reproduction of experimental results is quite good.

Some important points:

1. *f* electrons in the unfilled *f* shell in the paramagnetic ion form highly correlated f^n electronic subsystem due to Coulomb and spin-orbit interactions.
2. all paramagnetic ions, having an unfilled shell like 4*f*, 5*f* or 3*d*, can be divided with respect to the number of involved electrons into two classes: non-Kramers (an even number of electrons) and Kramers systems with an odd number of involved electrons; these two classes exhibit different behavior in the external electric field, namely with respect to the formed ground state. For the Kramers system the charge (electrostatic or electric-field made) ground state is always Kramers doublet that can be only split by external magnetic field or by spin-dependent (electrodynamic) interactions,
3. In an intermetallic compound, containing paramagnetic ions, there coexists band/itinerant electron and localized electrons; in order to account for this situation the individualized-electron model is worked out for intermetallics; these two subsystems are described by different theoretical approaches,
4. interactions of these two subsystems proceed via the charge and spin interactions; in most cases the low-energy excitations, below 0.5 eV, are spin-involved excitations,
5. the magnetic moment of an ion is not constant value; the ionic moment in a solid depends on the electric and magnetic fields in which the ion is placed; this effect is known in conventional compounds as a suppression of the local moment by CEF interactions,
6. there is no direct correlation between the low-temperature ordered moment and the high-temperature effective moment; the first is related with the $\langle J_z \rangle$ value of the ground state whereas the later reflects the J value of the ground multiplet,
7. the excitations of the f^n subsystem are many-electron excitations in contrary to single-electron excitations proceeding in the conduction bands; f^n excitations are neutral and spin-involved excitations,
8. excitations of the f^n system can be of very small energy being probed in low-temperature specific-heat experiments though their states are lying energetically much below the Fermi level;
9. the excitation level passes through the Fermi level of the conduction electrons, the ground state of the *f* electron system and the nuclear ground

state,

10. the CEF approach with S-D interactions, in the mean-field approximation, is able to reproduce, among others, the value of the local magnetic moment, value of the magnetic ordering temperature, temperature dependence of the local moment, of the magnetic susceptibility, of the specific heat, of inelastic-neutron-scattering excitations.
11. for reliable discussion of magnetic and electronic properties of any 4*f* /5*f* containing compound all CEF terms have to be taken into account; higher-order terms play important role in formation of the ground state of the *f* subsystem that determines the low-temperature properties.

III. TOWARDS HEAVY-FERMION PHENOMENA: THE CRYSTAL-FIELD AND KONDO-EFFECT MODEL

In the presented view, the heavy-fermion behavior is expected for (intermetallic and ionic) compounds containing Kramers ions, like f^1 (Ce^{3+}), f^{13} (Yb^{3+}), f^3 (Nd^{3+}, U^{3+} and Np^{4+}), f^5 (Sm^{3+} and Pu^{3+}). All of these systems have Kramers doublet as the charge-formed (CF) ground state. The removal of the Kramers degeneracy, due to spin-dependent interactions, is essential point for the understanding of h-f phenomena.

In these compounds CF Kramers doublet ground state is only slightly split. A small splitting of the Kramers doublet, of order of few K or a few tens of K, can be realized in solids if spin-dependent interactions are weak or the charge-formed ground state is weakly magnetic. The *f* ions, in such weak magnetic states, hardly enter into exchange interactions as then the system hardly gains the magnetic energy. An *f* intermetallic system with the CF ground state for the *f* electronic subsystem close to the N-M Kramers doublet exhibits remarkable properties of physical importance like a non-magnetic low-temperature state, a largely enhanced susceptibility, the substantial anisotropy of magnetic properties and the smooth transformation with temperature from a non-magnetic h-f state to the localized-moment state, inferred from a Curie-Weiss-like behavior of the paramagnetic susceptibility, Fig. 8 [19]. These properties are just the main characteristic features of compounds known as by h-f compounds.

The effect of charge and S-D interactions on the localized atomic-like *f* states leading to the splitting of the Kramers-doublet ground state is illustrated in Figs 2, 4 and 6. The charge and S-D interactions are approximated by the crystalline-electric-field (CEF) and molecular-field (MF) approaches.

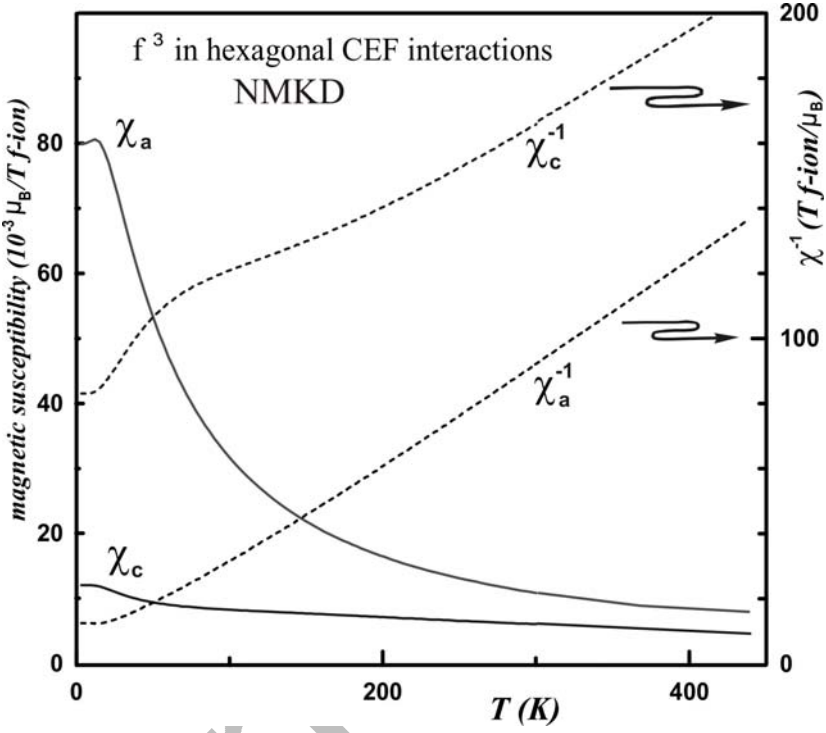

Fig. 8. Temperature dependence of the single-ion susceptibility for the f^3 configuration with the non-magnetic Kramers doublet state. It shows a non-magnetic behavior at low temperatures (for both directions!!) and conventional Curie-Weiss behavior at high temperatures. Similar behavior is observed in h-f compounds. After ref. 19.

These two interactions lead to a **magnetic singlet ground state** of the f^n system. It is important to realize that the Kramers degeneracy can be only removed by S-D interactions. The Kramers degeneracy **has to** be lifted out before T = 0 K, otherwise the 3rd thermodynamic law will be violated. This effect resembles the Jahn-Teller effect occurring for non-Kramers systems. Interesting phenomena occur if the system has difficulty in the removal of the Kramers degeneracy. This can happen if S-D interactions are weak or the charge-formed ground state is only weakly magnetic what is obvious looking at a Heisenberg-like Hamiltonian that the effect of S-D interactions depends

on the value of the exchange integral and of the considered spins. An almost non-magnetic local state can be formed by the highly anisotropic charge distribution that is manifest by higher-order CEF interactions [19,20]. **The effect of the anisotropic charge distribution of conduction electrons on the ground state of the f^n subsystem has not been considered in other existing models** (i.e. the Anderson, Hubbard or Kondo Hamiltonians). In the Kondo picture the local moment is compensated by oppositely oriented spins of conduction electrons whereas the electronic cloud of conduction electrons is considered to be isotropic. In the h-f hybridization models details of conduction-electron distribution are not discussed and the local magnetic moment is lost by hopping of the magnetic electrons to the conduction band.

Low-temperature moment *vs* high-temperature moment: There is no correlation between value of the local moment derived in the low-temperature magnetically-ordered state and the effective moment derived from temperature dependence of the magnetic susceptibility in the paramagnetic state. In ref. 19 it has been shown that the susceptibility curves with the zero-value of the low-temperature moment show normal Curie-Weiss behavior in the paramagnetic state, Fig. 8. It is presently obvious that the low-temperature moment is associated with the moment of the ground state whereas high-temperature susceptibility carries information about all CEF levels that are determined by the value *J* of the lowest multiplet.

The large low-temperature specific heat: The lifting of the Kramers degeneracy and the appearance of the localized state very close to the ground state results in a great number of low-energy excitations observed in specific-heat experiments as enormous heat consumption at lowest temperatures. The smaller splitting δ the lower temperature region with the large specific heat. This large low-temperature specific heat is one of the most prominent, and in fact historically original, characteristics of heavy-fermion compounds. Despite of details of the removal of the Kramers degeneracy, and associated with it details of temperature dependence of the specific heat, the overall low-temperature entropy is always $k_B \ln 2$ per atom. The large low-temperature specific heat and the associated entropy of $R \ln 2$ (per mole) are in agreement with many, if not all, experimental observations for h-f compounds.

***f* states *vs* *f* excitations**: From the discussion of the specific heat results and the Fig. 5 it is clear that *f* bound states are lying much below the Fermi level, 2-8 eV, but excitation-energies of the *f* subsystem can be very low, even below 0.1 meV and subsequently *f* excitations can occur at very low temperatures, below 1 K. In other words, occurrence of large low temperature

specific heat does not directly mean the large density of states (of single electron) at E_F. The problem of the *f* states and *f* excitations seems to be very trivial, but it is not as lack of this differentiation was probably a reason for calling for the delocalization of the *f* electrons. The provided here explanation removes, at least partly, also a problem of the renormalization where it is necessary to shift the calculated spectra obtained in the band-structure fashion in order to get agreement with experimental observations. The excitation level can have a meaning of the extended Fermi level if one thinks about the excitations in terms of quasiparticles. Most theoretical papers, if not all, deal with quasiparticles and it is probably one of the misleading point between experimentalists and theoreticians as the discussed quasiparticles are usually not well-specified.

A small local magnetic moment: The appearance of the splitting of the Kramers-doublet ground state marks the appearance of the local internal field, and subsequently the appearance of the local magnetic moment (there is no longer full cancellation of the two opposite contribution from the Kramers conjugate-states that occurs in the paramagnetic region, fig. 9a). The local moment, i.e. the moment of the Kramers sublevel, can be quite small as an effect of the anisotropic charge distribution [19]. Even zero-value state have been obtained within ordinary CEF approach. However, the general symmetry considerations indicate that Kramers ions at 0 K have **always** a non-vanishing local moment and that the zero-temperature ground state of any system containing Kramers systems is a magnetic singlet. Namely, the Kramers degeneracy has to be removed before the system reaches the absolute zero temperature. This prediction about the magnetic ground state is in good agreement with recent experimental observations. More and more detailed studies of h-f compounds reveal its magnetic ground state, even in compounds like $CeAl_3$ [8,28] that by years has been known as prototype of the non-magnetic h-f compound. So small local moments as 0.03 μ_B are accepted at present to exist in URu_2Si_2 or UPt_3. This small-moment magnetism is nowadays revealed by microscopic-scale techniques like NMR, Mössbauer and μ^+SR are of great importance. In particular, the muon spectroscopy, a rapidly developing technique in last years, provides new insight into this ultra-small magnetism [29].

Weakly-magnetic Kramers doublet state is formed by CEF interactions due to the hybridization of the atomic states $|J,J_z>$ with opposite moment contributions as is seen from the explicit form of the non-magnetic Kramers doublet state [19,20]:

$$|\Gamma_9^1> = 0.86|\pm 3/2> + 0.5|\mp 9/2>.$$

This state is formed by CEF interactions of hexagonal symmetry due to the hybridization of the different atomic-like states $|J,J_z>$ as an CEF effect. All components of the magnetic moment $<\Gamma|J_i|\Gamma>$ of this Kramers state are zero. The susceptibility of the f^3 system with this ground state has been shown in Fig. 8. In [19,20] it is proved that this state can be realized as the ground state. The moment contribution of the state |-9/2> is opposite to the contribution of the state |+3/2>. It means that the weakly-magnetic state is due to cancellation of two quite big contributions. Also here we meet the effect of cancellation of the orbital and spin moment though in description of *f* magnetism we are usually using only the total angular momentum operator. Moreover, the small magnetic moment and small expectation values $<J_i>$ does not mean that the spin values are small. Due to this fact weakly-magnetic ground state can enter into spin-spin interactions.

Thermally-induced local spin fluctuations and their propagation in the lattice: The magnetic moment associated with the two Kramers conjugate states have the opposite value provided exchange interactions are weak. Strong S-D interactions destroy this symmetry. Weak S-D interactions preserve largely this symmetry. Thus, in case of weak S-D interactions the thermal excitation to the Kramers conjugate-state implies the reversal of the local magnetic moment and subsequently implies the reversal of the oscillatory polarization of the spin density associated with conduction electrons (see Fig. 9c). The mechanism for the formation of the oscillatory spin polarization has been found in the RKKY interactions. The local magnetic moment (with largely reduced, by a CEF-like effect, value compared to that of the effective moment in the paramagnetic region) and the spin-density polarization of conduction electrons, which is antiferromagnetically bound to it by means of the Kondo-type interactions, can be considered as the h-f quasiparticle. A thermally-induced local excitation to the Kramers conjugate state propagates through the lattice despite that their part - the *f* electrons - are staying localized, similarly to the situation in the standing waves in acoustics, Fig. 10. Although the description of thermodynamics of such processes is complex and complex will be temperature dependence of the specific heat their energies are comparable with δ that can be so small as part of Kelvin.

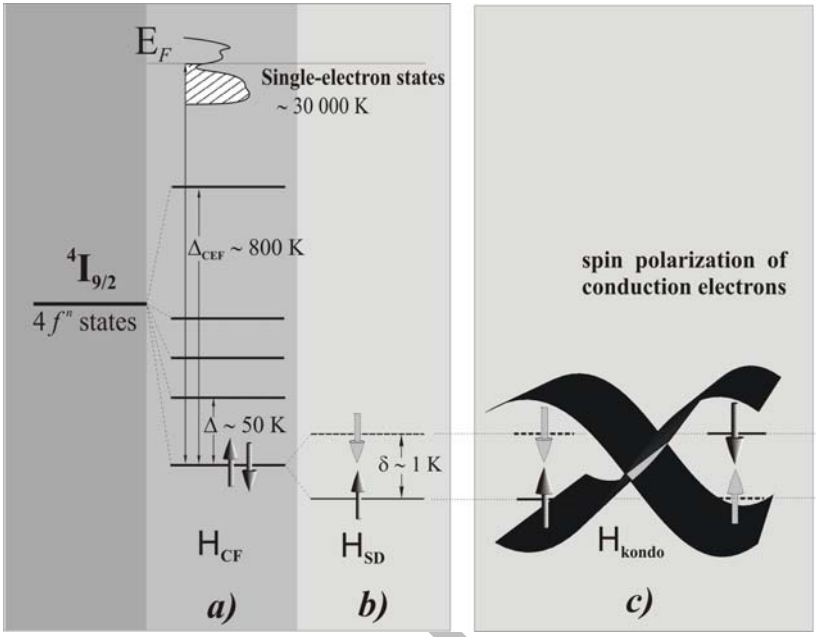

Fig. 9. The fine electronic structure of the ground multiplet of the f^3 Kramers system with realistic values for the energy splittings. The bound *f* states lie much below the Fermi level E_F. The ground multiplet $^4I_{9/2}$ is split by charge interactions H_{CF} into 5 charge-formed Kramers doublets, as shown in (a), which are subsequently split by spin-dependent interactions H_{SD} (b) (only the splitting of the ground state is shown). If S-D interactions are weak, the splitting of the Kramers doublet ground state is small and the local moment associated with two Kramers twin states have the opposite directions. The local magnetic moment of the CF ground state is largely suppressed as an effect of the anisotropic charge distribution, mainly of conduction electrons, at the vicinity of the *f* shell. c) The local moment causes the spin-polarization of conduction electrons whereas the Kondo-type interactions bind this spin polarization antiparallelly to the local moment. A thermal excitation to the Kramers conjugate-state causes the reversal of the local moment implying the reversal of the spin-polarization of conduction electrons. Such thermally-induced quasiparticles can propagate through the lattice though *f* electrons stay localized as is illustrated in (c) for two collective states of the local moment and the c-e spin polarization shown by solid and dashed lines. Notice, that (a)

refer to the paramagnetic state, whereas (b) and (c) to the magnetic state. At any temperature and at given site only one state of the Kramers doublet is occupied. The on-site antiferromagnetic (AF) fluctuations as well as inter-site AF correlations between the local moments at neighbouring sites should be noticed.

δ and Δ denote the splitting of the Kramers-doublet ground state and the separation to the first excited CEF level. δ and Δ introduces in the system two energy scales.

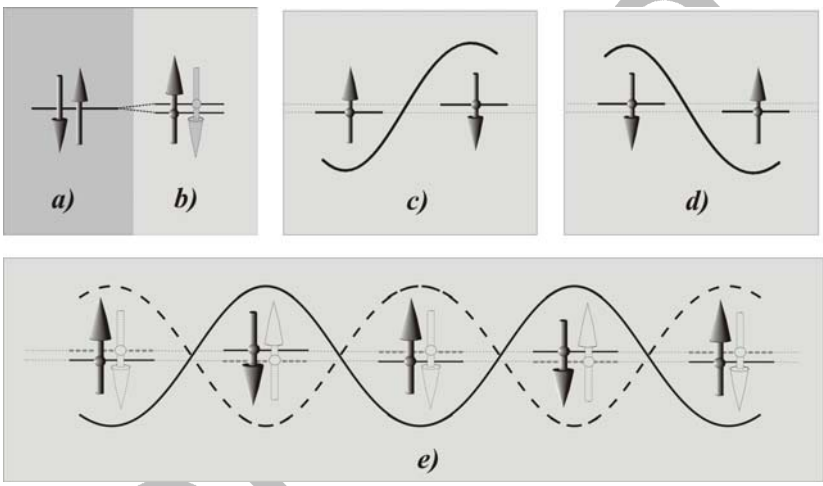

Fig. 10. The propagation of the spin-waves in the lattice sites due to the thermal excitation to the Kramers conjugate state, the moment (spin) of which is opposite. See also the caption of Fig. 9.

Quasiparticles: in this picture the h-f particle is associated with the f^n fermion (n is an odd number: n=1 corresponds to the Ce^{3+} ion, n=3 - to the Nd^{3+} ion and U^{3+} ion, n=13 corresponding to the Yb^{3+} ion behaves as a 1-hole system) dressed with conduction electrons by spin interactions; in fact, the h-f particles are neutral many-electron spin-involved excitations associated with two closely-lying localized states of the f^n strongly - correlated electron subsystem; it is interesting to note, that such quasiparticles behave like bozons as they are associated with local excitations at each ion; at zero temperature

the each ion is in the localized singlet ground state. Such view is in sharp contrast to charge excitations considered in the hybridization models; in the Fermi liquid model, for instance, the quasiparticle is considered as the complex consisting of an electron and its rearrangement cloud that moves much more slowly than a free electron of the same energy. Such interpretation is clearly stated in ref. [30] where one can also read "below T^* the 4f-electron must be considered as partially delocalized because a heavy-fermion liquid forms". To make it clear, in the presented view there is no delocalization of the 4f-electron. My localized point of view is supported by quite recent studies [31] showing that "in contrary to the one-particle picture, the heavy quasiparticles may be viewed as loosely bound states of conduction electrons and spin-wave-like excitations of the nearly localized *f*-electron system". I fully agree with this conclusion trying to minimalize the meaning of the word "nearly". This small word is not an academic discussion. The deviation of the occupation of the *f* states, n_f, from the integer number determines in the Landau-Fermi liquid model as well as in the renormalized-band theory [2,30] the h-f behaviour.

On-site AF fluctuations: The existence of the two Kramers twin localized states with the opposite-moment direction in case of weak S-D interactions allows for an interesting phenomenon that can be called **on-site antiferromagnetic fluctuations**. This effect is clearly visible in fig. 9b and 10. It is worth to note that in $NdNi_5$ such on-site AF fluctuations are already not realized [32], Fig. 11. Apparently S-D interactions are already too strong though T_c amounts to 7.2 K only. This example shows that S-D interactions have to be weak indeed for the occurrence of the thermally-induced on-site AF fluctuations. We could simulated this behavior taking CEF and S-D interactions such to produce the local moment 0.4 μ_B and T_c of 1 K only, Fig. 12a. On Fig. 12b the temperature dependence of the magnetic moment associated with two Kramers conjugate states shows that two moment are of the opposite direction. Note that this AF fluctuations occur in $NdNi_5$ at temperatures close to T_c as one can see from Fig. 11. Figs 11-12 illustrate the formation of the local magnetic moment for the Kramers system.

The heavy-fermion state: It is a magnetic state with weak intersite magnetic interactions. The source of the magnetism are paramagnetic ions with an odd number of strongly-correlated electrons. This state is formed by time-reversal symmetry breaking. A local magnetic moment of the 4f shell is the order parameter as it appears after this breaking. Although there is the doublet ground state and it is associated with the spin-degree of freedom it

behaviour is complex, namely it cannot be approximated by an effective spin of 1/2.

Two energy scales in the system are introduced by the presence of the splittings δ and Δ. The splitting of the ground state Kramers doublet δ predominantly governs the low-temperature specific heat. The smaller δ the larger low-temperature specific heat. Many magnetic and electronic

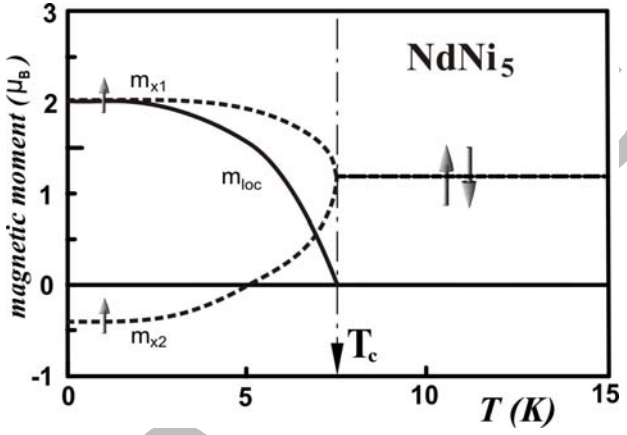

Fig. 11. Temperature dependence of the local magnetic moment (m_{loc}) and the moments associated with two Kramers conjugate-levels m_{z1} and m_{z2} calculated with the parameters relevant for $NdNi_5$, a conventional ferromagnet with T_c of 7.2 K, with parameters B_2^0=+3.35K, B_4^0=+14.5mK, B_6^0= -0.35mK, B_6^6= -13.5mK and n=3.5 T/μ_B. Magnetic moments associated with two Kramers conjugate-states have the opposite sign (note that for the moment m_{z2} the left scale should be used) that cancel exactly in the paramagnetic state. In the ordered state the value of the local moment increases due to the increasing difference in the population of the two Kramers conjugate-states (mainly) and increasing difference of their values. Below 5 K there is no reversal of the moment as the moments associated with two Kramers conjugate-states have the same direction illustrating the case of strong S-D interactions where the moment assymetry is fully broken. Compare with the next figure where the case of the weak S-D interaction is shown. After Ref. 22.

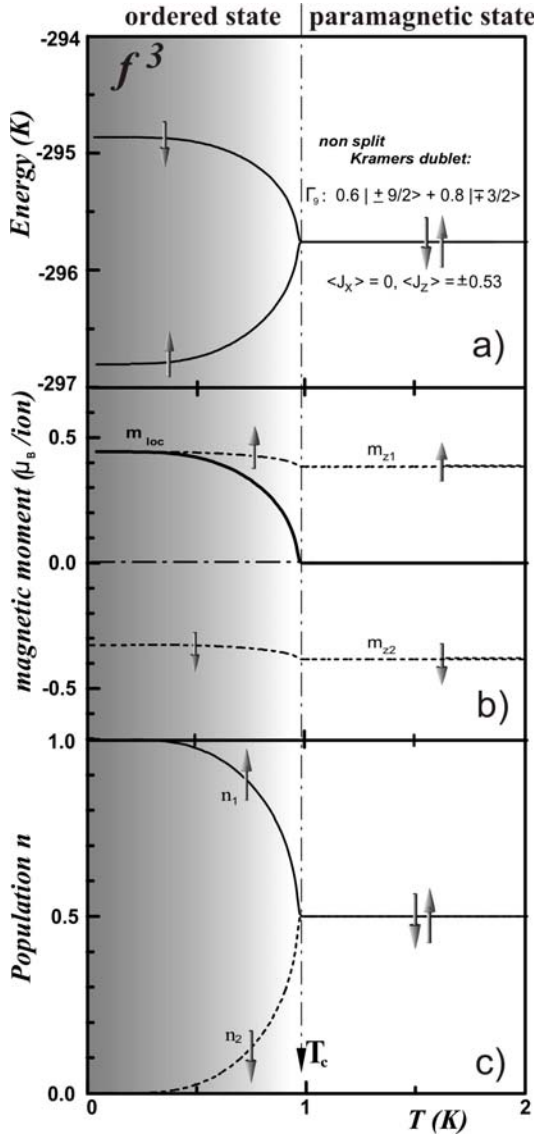

Fig. 12 a) The splitting of the CF ground state Γ_9 of the f^3 Kramers system by weak S-D interactions below T_o of 1.0 K simulated by a set of CEF parameters of the hexagonal symmetry: B_2^0 = +4.5 K, B_4^0=-123 mK,B_6^0= -2 mK, B_6^6=-52.3 mK and n of 8.5 T/μ_B. The ground state Γ_9 has weak magnetic characteristics with expectation values of $\langle J_z \rangle = \pm 0.53$ and $\langle J_x \rangle = 0$. Arrows indicate the direction of the magnetic moment associated with each local state.

b) Temperature dependence of the local magnetic moment (m_{loc}) and the moments associated with two Kramers conjugate-levels m_{z1} and m_{z2} calculated with the parameters listed above. This figure illustrates the case of weak S-D interactions where the moments of Kramers conjugate states become different but remaining in opposite directions.

c) the temperature dependence of the population of two Kramers conjugate states. The population is governed by Boltzmann-distribution function.

properties exhibit some anomalies at temperatures compared with the energy separation to the first excited state Δ. This anomaly is more visible if other excited states are much higher. The specific heat, for instance, exhibits a Schottky-type maximum at temperature about 0.42Δ. The anomalous temperature dependence of the quadrupole 4*f* moment and the electric-field gradient with a maximum has been calculated for $NdNi_5$ [22] and $YbCu_2Si_2$ [33] within this approach reproducing very well experimental Mössbauer data [34]. Thus in the present model **the splitting δ of the ground-state Kramers doublet corresponds to the width of the Kondo resonance peak whereas Kondo temperature is associated with the separation to the first excited CEF level.** For instance, the Kondo temperature for $YbCu_2Si_2$ has been evaluated for 200 K [35, 36] whereas the separation to the first excited level found by inelastic-neutron-scattering studies amounts to 17.6 meV (=210 K) [37]. The Kondo-anomaly is more visible if the number of involved CEF levels is smaller and they are well separated as is in case of Ce^{3+} ion (3 Kramers doublets), Yb^{3+} (4 Kramers doublets) or Nd^{3+}/U^{3+} (5 Kramers doublets).

Resistivity: in this model large anomalies in the temperature dependence of the resistivity are not associated with changing the number of carriers but with large changes in the scattering form factor. New scattering channels are opened if temperatures fit to the CEF excitations provided non-vanishing matrix elements for the scattering process. The anomalies are more visible in case of small number of levels. This explanation is supported by the fact that always resistivity of a *f* intermetallic compound is larger than the reference Y/La system, see Ref. [38], where the temperature dependence of the resistivity of UBe_{13} and YBe_{13} is presented. The larger resistivity in *f* intermetallics surely does not indicate the larger number of carriers as is supposed in the hybridization models. In contrary, this indicates smaller number of carriers or predominantly changes of the scattering process of conduction electrons on the lattice ions. The smaller number of carriers is strong argument against the delocalization of the *f* electrons. Such increase of the resistivity for the 4*f*-containing compounds compared with La or Y compounds is the general observation and is associated with the presence of great number of independent (loosely-bound) scattering centers. Frequently found a T^2 dependence at low temperatures, taken as a strong argument for Landau-Fermi liquid theory, seems to be meaningless as it is a very-short temperature-interval property and the lowering of the resistivity going to zero

temperature is characteristic for the formation of the collective magnetic state. Moreover, measurements on single-crystalline $CeAl_3$ [39] reveal i) the large anisotropy of the resistivity and ii) a T^4 dependence instead of the T^2-dependence. These effects cannot be accounted for by the present versions of the Landau-Fermi and Kondo-lattice models.

Photoemission: According to the present model the large density of states close to E_F detected in photoemission spectroscopy is related with many-electron localized excitations over the fine electronic structure originated from the *f* ion. The photon before knocking out a photoelectron lose some energy in local interaction with the *f* ion causing its excitation to a f^{n*} state, where f^{n*} denotes an excited state that can be in the same manifold (an involved energy up to, say, 30 meV) or in other multiplet (an involved energy of about 500 meV). Thus the photoelectron has the lower energy by the CEF/multiplet energy. In photoemission experiments they are detected below E_F. This interpretation of the EPS spectra is in agreement with those proposed by Joyce et al. [40].

IV. Consequences and predictions of the CEF and Kondo-effect model:

1. Heavy-fermion phenomena can occur for compounds containing Kramers systems, both in intermetallic and ionic compounds,
2. The Kramers system is a system of an odd number n of electrons/ fermions which are highly correlated. Their physical realization one meets in paramagnetic ions with unfilled d or *f* shells,
3. The Kramers system f^n is a (heavy-)fermion; these fermions (Kramers systems) follow the Bose-Einstein statistics as they are located at different ions (localized),
4. the CEF approach is the simplest, but physically adequant, approach that takes into account very strong correlations of electrons due to Coulomb interactions and spin-orbit interactions. Taking into account in CEF calculations the spin-orbit interactions allows to call CEF interactions as relativistic calculations. Moreover, CEF calculations are taking into account the orbital magnetic moment being in this point superior to standard band-structure calculations.

Some consequences and predictions are following:

1. the low-temperature heat entropy ----- Rln2
2. the small splitting δ (<0.1 meV)---- a lot of low-energy excitations at ultra-low temperatures,

3. the smaller spin-dependent interactions the smaller δ; the smaller δ the bigger low-temperature specific heat,
4. the local ground state is always magnetic though the local moment can be very small; it causes always a magnetic (spin-wave) ground state at the absolute-zero temperature,
5. a smooth transformation of the low-temperature h-f state into the local-moment regime at ambient temperatures,
6. the nonzero magnetic moment in the local atomic scale (in contrary to the Kondo effect),
7. large anisotropy of magnetic, electronic and transport properties,
8. local antiferromagnetic fluctuations are very natural in the Kramers system; they are between two conjugate Kramers states,
9. the model easily explains the occurrence of the h-f behavior in ionic systems like a low-carrier compound Sm_3Se_4 or high-T_c superconductor $Nd_{1.8}Ce_{0.2}CuO_4$,
10. the (spin) interactions of the *f* subsystem and conduction electrons is weak; this point is opposite to the assumption of the existing models dealing nowadays strongly-correlated electron systems,
11. in this model strong correlations occur between the *f* electrons; the *f* electron subsystem is a strongly-correlated electron system f^n and it is the fermion,
12. The model is well founded in solid state physics,
13. The model can be extended to Kramers d^n systems of 3*d* paramagnetic ions; in fact, the first heavy-fermion like behaviour has been found in diluted 3*d* alloys already 50 years ago,
14. The model can be extended to nuclear Kramers systems; here first of all ^{3}He should be mentioned; it exhibits large specific heat at temperatures below 0.5 K,
15. The localized character of *f* electrons does not contrast with collective nature of the magnetism and superconductivity; the localized *f* electrons are taking part in spin waves.

In view of the present model, the heavy-fermion phenomena can occur for compounds containing a Kramers system. The h-f behavior is related with difficulties in the removal of the Kramers degeneracy, that **has to be removed** before T = 0 K. The ground state of the f^n Kramers system is always **magnetic** though the associated magnetic moment can be extremely small. The thermally-induced local excitation to the Kramers conjugate-state causes the reversal of the local magnetic moment implying subsequently, due to the

Kondo coupling, the reversal of the oscillatory polarization of the conduction-electron spin density. Such the bound many-body excitation, the h-f quasiparticle, can propagate through the lattice though the *f* electrons are staying localized. Due to this subsequent reversal mechanism the local excitation is no any longer a local event and leads to an effective coupling of the local spin with the lattice. Judging the present model one should note that 1) the original Kondo-impurity model starts from the localized impurity states, 2) the Kramers-doublet ground state has been determined for such prominent h-f compound as UBe_{13} [41], 3) the localized states have been observed in inelastic-neutron-experiments for such h-f compounds as UPt_3 [42] and URu_2Si_2 [43]), 4) more and more magnetic ground states are revealed for h-f compounds by the muon spectroscopy, 5) the trivalent uranium state has been revealed in so prominent h-f compounds like UPt_3, UBe_{13} and $CeCu_2Si_2$ by X-ray studies of the local form factor [44] and the single-ion behaviour of the susceptibility as been found in UBe_{13} by studying the Y dilution [38].

The present model is, somehow, in spirit of the lattice of the Kondo single-impurities (it is not equivalent to a model presently known as the Kondo-lattice model) in which impurity states are localized but in which the Nozieres objection [15] has been overcome as the local moment is predominantly suppressed by the charge CEF-like mechanism but not by the spin-compensation mechanism. According to the present model, and in contrary to the hybridization model, the conduction electrons are not indispensable for the occurrence of h-f phenomena. Thus, the present model offers explanation for ionic compounds and low-carrier h-f systems, like Sm_3Se_4 [45] or $Nd_{1.8}Ce_{0.2}CuO_4$ [46], that exhibit heavy-fermion phenomena without the Fermi surface. This model seems to be also applicable to ^3He, that can be considered as an nuclear Kramers system [32].

Analysis of large specific heat of $Nd_{2-y}Ce_yCuO_4$ has been given in ref. [47]. It is proved there that the large specific heat in Nd_2CuO_4 occurring below 3 K is due to the removal Kramers degeneracy of the Nd^{3+} ion. The splitting δ amounts to less than 0.5 meV. Such small splitting is caused by almost cancellation at the Nd site of the molecular fields originating from (antiferromagnetically) aligned Cu-ion moments.

Further insight into possible magnetic state developed in the h-f state: In a spin-wave state one expects that the molecular field acting on the *f* shell varies from site to site. It causes the site variation of the splitting δ. As a consequence, the specific heat is a convolution of the Schottky-type contributions with different splittings δ. In well-developed ferro- and

antiferromagnetic states the molecular field and the splitting δ is constant through the lattice-ion as it is in $ErNi_5$ or $NdNi_5$. This distribution of δ over different sites has the similar effect on the specific heat as the broadening of CEF levels. Thus the found broadening of CEF levels in YbBiPt [48], by careful analysis of specific-heat data, can equally have the distribution of δ over the lattice sites in origin.

CEF approach and band structure calculations: It is necessary to remark that though the description of the localized states is here given in frame of the CEF and MF model, the conclusion about the removal of the degeneracy of the bound electronic *f* states is not affected by limitations of CEF and MF approaches. These conclusions are based on the general-symmetry considerations, namely the time-reversal symmetry and the 3rd thermodynamic law. Values for the CEF parameters themselves are the subject of the discussion but band-structure calculations will have to reproduce the found energy separation and magnetic characteristics of the ground state. It will be possible if band structure calculations reaches the required accuracy; the band-structure calculations give at present the electronic structure with the accuracy of 0.5 eV, i.e. of 5 000 K. Discussed here effects are more than three orders of magnitude smaller. Moreover, it should be noted that CEF calculations incorporate from the beginning the relativistic effect of spin-orbit interactions - band-structure calculations provide usually the spin-only part and have enormous difficulty to take into account spin-orbit coupling. But it is known that spin-orbit coupling increases with increasing Z value. So meaningful band-structure calculations for heavy ions have to take into account spin-orbit interactions. Due to this point even approximate CEF calculations provide more reliable physical description of low-energy neutral excitations than the present band-stucture calculations. Moreover, the presently available band-structure calculations and the Landau-Fermi-liquid description provide information close to the absolute zero-temperature.

V. Conclusions.

The understanding of the heavy-fermion compounds has been proposed within concepts developed for conventional rare-earth intermetallic compounds where *f* electrons are taken to be fully localized. The large low-temperature specific heat and other h-f-like phenomena are expected for compounds containing Kramers systems. The Kramers system it is a strongly-correlated electronic system with an odd number of electrons (in general fermions). The h-f-like behavior is related with difficulties in the removal of

the Kramers degeneracy of the localized *f* states that causes that the splitting δ of the Kramers-doublet ground state is small, even of order of 0.1 meV. This model belongs to class of spin-transfer model like the original Kondo single-impurity model but in contrary to the Kondo model takes into account the suppression of the local moment via the anisotropic charge distribution. This model can be experimentally distinguished from the original Kondo-lattice model by local atomic-scale techniques like Mössbauer and NMR spectroscopy. In the Kondo-lattice model there exists the local atomic-scale magnetic moment of substantial size comparable with that seen in the paramagnetic state whereas in the presented model the local atomic moment is small. The removal of the Kramers degeneracy, that has to occur before the system reaches the absolute zero temperature, causes the appearance of two closely-lying many-electron states with the oppositely oriented local magnetic moment. Then thermal excitation to the Kramers conjugate state causes the reversal of the local magnetic moment and subsequently, due to the Kondo-like Hamiltonian, pulls the reversal of the oscillatory spin polarization of conduction electrons. By involving this local-spin fluctuation mechanism the local thermal excitation is not longer the local event because it pulls a collective excitation in form of spin-density waves through the lattice.

In this approach we treat the paramagnetic ion as a microscale probe. By studying the ground state of the paramagnetic ion we can learn about the charge and spin distribution in the lattice. Of course, there is influence of the local charge and spin on the ground state of conduction electrons finally leading to the self-consistent total ground state. This model can be understood as our view that for the physically adequate description of magnetic and electronic properties of any 4*f* /5*f* compound crystal-field interactions have to be clarified and evaluated the first.

The concept that the *f* electrons are localized in compounds exhibiting h-f phenomena is nowadays highly unpopular within the h-f community but it is a matter of further theoretical analyses of experimental results to see how far this approach, in particular the underlying of the well localization of the *f* electrons, is useful for *f* intermetallics including those exhibiting h-f phenomena. There is rapidly growing number of compounds, like UGa_2 [24], UPd_2Al_3 [26,27] or YbBiPt[48], properties of which can be consistently understood within the individualized-electron taking the *f*-electrons to be localized. The author is convinced that there is no conflict of this theory with most modern theoretical approaches. The present theory discusses the microscopic physical origin of the h-f phenomena in contrary to the other

approaches that are largely phenomenological. Many of spin-fluctuation approaches seem to be directly applicable to this new view on h-f problem.

The proposed theory is well founded on the existing concepts of the solid state physics, including interaction of the localized spin with conduction electrons (Kondo Hamiltonian). It belongs to spin-transfer models. It clearly reveals difficulties in description of the heavy-fermion state as it is a state involving energies even below 0.1 meV. The model deals with such small energy separations associating them with the fine electronic structure allowing simultaneously for bridging the solid state physics with the atomic physics. It is the first model that consistently explains low-temperature and high-temperature properties of heavy-fermion compounds independently on their metallic or ionic behavior. Moreover, the localized *f*-electron approach is well founded in metal physics of conventional *f* intermetallics and is simple. As "The simple is the seal of the true" (an ancient motto [49]) it is believed that this approach really help to understand the h-f phenomena.

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