Physics of strong electron correlations: YbRh₂Si₂, CeRh₂Si₂, NiO and Ba₂IrO₄

R. J. Radwanski,^{1,2} D. M. Nalecz,¹ and Z. Ropka²

¹Institute of Physics, Pedagogical University, 30-084 Krakow, Poland ²Center of Solid State Physics, S^{nt}Filip 5, 31-150 Krakow, Poland

Strong electron correlations occur very often in the modern solid-state physics and chemistry, quantum and classical. They are charged to be a reason, in fact, for everything. Strong correlations are, for instance, charged to be a reason of unability of the first-principles studies based on the local density approximation (LDA) to describe the insulating ground state of 3d/4f oxides. Also strong correlations are regarded to be a reason for heavy-fermion (h-f) phenomena in Ce, Yb or U intermetallics. Despite of their occurrence in most of scientific papers we feel that their physical meaning is quite physically undescribed. The aim of the present contribution is to clarify the predominant origin of strong electron correlations in transition-metal compounds, i.e. compounds containing 3d/4f/5f/4d/5d atoms, in particular with respect to the on-site or the intersite correlations. We claim a substantial physical importance of the on-site electron correlations. In all titled compounds there is growing experimental evidence for realization of Yb^{3+} , Ce^{3+} , Ni^{2+} and Ir^{4+} ions with integer number of electrons in the open-electron shell forming $4f^{13}$, $4f^1$, $3d^8$ and $5d^5$ strongly-correlated quantum systems, respectively. We are fully aware that our scientific point of view is in sharp contrast to widely spread view that h-f phenomena are associated with strong mixed valence and/or strong hybridization of localized f electrons with conduction electrons. In our view this large specific heat at low temperatures originates from difficulties in the removal of the ionic Kramers-doublet ground state. In last years crystal-field Kramers-doublet states have been revealed in profound h-f YbRh₂Si₂ and CeRh₂Si₂ intermetallics. According to us the h-f excitations are spin-like charge-neutral lowenergy excitations, (< 0.2 meV), in contrary to charge excitations expected by the hybridization Fermi-liquid mechanism.

For NiO the value of the magnetic moment and its direction have been reproduced taking into account the crystal-field and spin-orbit interactions. The fine-electronic structure in Ba_2IrO_4 is governed by the intra-ionic spin-orbit coupling. Finally we would like to point out that the formation of ions, with realization of localized discrete energy states, close to the Fermi level, is manifestation of on-site strong-electron correlations. The presented view is in line with Georges et al. [Ann.Rev.Cond.Mat.Phys. 4 (2013) 137; arXiv:1207.3033v2] who pointed out that the Hund's rule coupling (intraatomic exchange) is responsible for strong electron correlations. We would like to note that one of us (RJR) already 25 years ago pointed out the importance of crystal-field and spin-orbit interactions, obviously acting on Hund's rules physics, for theoretical description of magnetic and electronic properties of 3d/4f/5f/4d/5d compounds, both intermetallics and oxides.