Competition between the Kondo and the crystalline field effects of multi-electron ions, and attempt to calculate the band dispersion of heavy electron systems

O. Sakai ${ }^{1}$, R. Shiina ${ }^{1}$, Y. Kaneta ${ }^{2}$, Y. Shimizu ${ }^{3}$

1 - Department of Physics, Tokyo Metropolitan University, Minami-Ohsawa, Hachioji, Tokyo 192-0397, Japan
2 - Department of Quantum Engineering and System Science, University of Tokyo Tokyo, 113-8656, Japan
3 - Department of Applied Physics, Tohoku University
Sendai 980-8579, Japan
We calculate the magnetic susceptibility of ions with multi-electron occupancy on the basis of Anderson impurity model, which includes the crystalline electric field and Hund's rule coupling term. Wilson's numerical renormalization group method is used. The Kondo like singlet state with two holes bound state appears in a certain situation of the $\mathrm{f}^{2}$ configuration ion. There also appears the crystalline field singlet-like ground state with Kondo like behavior in high temperature region. In a restricted parameter case, we can expect the non-fermi liquid state of two-channel Kondo type even for the Anderson model which has local fermi liquid state in the non-interaction case. Characteristics of the temperature dependence of the susceptibility are shown.

We also show a method to calculate the energy band dispersion by applying the DMF method for the LMTO band calculation scheme. We show the results for $\gamma-C e$ and $\alpha-C e$. The attempt to application to multi-electron occupancy system is explained.


Fig. Temperature dependence of the normalized magnetization for several values of the magnetic field, $\mathrm{H}_{\mathrm{Z}}$. In A of the doublet-like case, $\ln T$ increase is seen in the region of $T \gg H_{Z}$. B is the CFS-like case, and C is the $\mathrm{f}^{0}$ like case near the quantum critical point between the fermi-liquid and the non-fermi-liquid states. D is the $\mathrm{f}^{0}$ like case. The data denoted by circles, diamonds and triangles in A and B are calculated for $\mathrm{H}_{\mathrm{Z}}=10^{-9}$, $10^{-8}$ and $10^{-7}$, respectively, and in C and D for $H_{\mathrm{Z}}=10^{-8}, 10^{-7}$ and $10^{-6}$.

