The interplay of $4f$ state and superconductivity in $CeIr_3$: DMFT study.

Sylwia Gutowska[1] and Bartłomiej Wiendlocha[1]

[1] *Faculty of Physics and Applied Computer Science, AGH University of Science and Technology in Krakow*

$CeIr_3$ has caught the attention over the past few years. It grows in trigonal structure and is a superconductor below $T_c = 3.1\,\mathrm{K}$. On the one hand the muon spin rotation and relaxation measurement shows its superconductivity to be of nearly BCS character [1], while on the other hand multiband character of this effect has been deduced from temperature dependence of critical magnetic field [2].

In our first work [3] we have shown, that its electronic band structure, including multiband Fermi surface, is dominated by Ir $5d$ states, thus their are suggested to be crucial for superconductivity of $CeIr_3$.

However, the role of $4f$ states of cerium is still unclear. If nearly BCS character of superconductivity is a case in $CeIr_3$, the McMillan formula for electron-phonon coupling (EPC) constant should be proper and resulted value 0.67 should agree with the EPC constant calculated as a renormalization of electronic part of heat capacity, $\lambda = \frac{\gamma_{expt}}{\gamma_{calc}} - 1$, where γ_{expt}, γ_{calc} are Sommerfeld constants determined on the basis of measured heat capacity and calculated electronic structure respectively. However, the result of letter formula is strongly dependent of a treatment of f states in calculations, being equal to 1.47 in the case of GGA approximation of electronic correlation and 3.40 in the case of GGA+U approximation. Both values are in strong disagreement with McMillan value, suggesting, that both approximations of electronic band structure of $CeIr_3$ fail and a role of $4f$ states is more subtle.

Here we are presenting the new approach to the band structure of $CeIr_3$ with help of embedded dynamical mean field theory (eDMFT) [4], which allows to treat f states properly. We show, that $4f$ states of Ce are present around the Fermi level more than previous study show, leading to smaller renormalization of heat capacity and a better agreement with McMillan value of EPC constant. This study show, that even if Ir $5d$ states are crucial for superconductivity of $CeIr_3$, Ce $4f$ states are also important, as they are present around Fermi level and are weakening the electron-phonon interactions.

References:

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