Neutron magnetic form factor in strongly correlated materials
MARIA PEZZOLI, KRISTJAN HAULE, GABRIEL KOTLIAR, Serin Physics Laboratory, Rutgers University,Piscataway, NJ 08854, USA. — We introduce a formalism to compute the neutron magnetic form factor $F(q)$ within a first-principles Density Functional Theory (DFT) + Dynamical Mean Field Theory (DMFT). We use our method to compute the form factor of $PuCoGa_5$. We find that the local physics of this material is described by a mixed valence mechanism of the type observed in elemental Plutonium. This picture explains nicely the experimental neutron form factor of $PuCoGa_5$ and it is consistent with the photo-emission spectra shape and the value of the specific heat linear coefficient.

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