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Spin-orbit coupling in three-orbital Kanamori impurity model and its relevance for transition-metal oxides

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The spin-orbit coupling (SOC) causes several effects: at the level of noninteracting electronic structure, it leads to the lifting of the band degeneracies and can induce a change of topology in the momentum space, a topic widely discussed today; in atoms, the SOC leads to the third Hunds rule; in magnetism, it leads to the spin-anisotropies.

We investigate properties of the three-orbital model with Kanamori and spin-orbit interactions at the impurity and dynamical mean-field theory (DMFT) level. Our investigation concludes that the SOC has no effects on the physical properties as long the orbital Kondo temperature is larger than the SOC.

We identify three regimes as we vary the SOC λ: the Hund's impurity for $|\lambda| < \lambda_c \approx T_{\mathrm{K}}^{\mathrm{orb}}$, van-Vleck non-magnetic impurity for $\lambda > \lambda_c$, and a $J = 2$ impurity for $\lambda < -\lambda_c$. All the regions correspond to a Fermi liquid but with very different quasiparticle phase-shifts.