First-principles analysis of heavy-electron superconductors

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Abstract:
Heavy-electron systems provide a unique playground to study novel quantum phases, such as complex magnetic / multipole order, unconventional superconductivity, and anomalous quantum criticality. However, in spite of intensive research efforts, most of these interesting phenomena have not been fully understood yet. This can be partly due to the complicated electronic structure, indispensable spin-orbit coupling, and also strong electron correlation. Recently, we have developed a procedure to evaluate several correlation functions based on the first-principles calculations [1]. This approach provides knowledge about higher-order multipole fluctuations. So far, we applied this analysis to URu_2Si_2 [1], $CeCu_2Si_2$ [2], and UPt_3 [3]. We discussed rank-5 order in URu_2Si_2, $s_{\pm}$-wave superconductivity in $CeCu_2Si_2$, and E_{2u} triplet pairing in UPt_3. In particular, related to the E_{2u} pairing, we have developed group-theoretical classification of multi-orbital superconductivity [4,5]. It indicates that symmetry of electron orbitals affect Cooper-pair symmetry [6]. In this talk, I will summarize these results and the remaining problems.

References:
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