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Slave Boson Theory of Orbital Differentiation with Crystal Field Effects: Application to UO_2 NICOLA LANATA, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA, YONGXIN YAO, Ames Laboratory-U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa IA 50011, USA, XIAOYU DENG, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08856-8019, USA, VLADIMIR DOBROSAVLJEVI, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08856-8019, USA — We derive an exact operatorial reformulation of the rotational invariant slave boson method and we apply it to describe the orbital differentiation in strongly correlated electron systems starting from first principles. The approach enables us to treat strong electron correlations, spin-orbit coupling and crystal field splittings on the same footing by exploiting the gauge invariance of the mean-field equations. We apply our theory to the archetypical nuclear fuel UO_2, and show that the ground state of this system displays a pronounced orbital differention within the $5f$ manifold, with Mott localized Γ_8 and extended Γ_7 electrons.

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