Orbital-selective Mott phase from a dehybridization in a multiorbital Hubbard model

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In multi-orbital systems, certain orbitals can become Mott localized, leading to an orbital-selective Mott phase (OSMP), which has been of interest to iron-based superconductors [1–3] and is also emerging to affect flat band physics [4]. Here, we consider the OSMP in the presence of an inter-orbital hopping term. The stability of the OSMP against an interorbital has been demonstrated using an auxiliary spin method [1–3], but has yet to be shown in methods based on the dynamical mean field theory [5]. In this work, we use the extended-DMFT (EDMFT) method so that inter-unit-cell correlation effects are taken into consideration. We solve the EDMFT equations with a continuous time quantum Monte Carlo method. An OSMP develops in the presence of the inter-unit-cell spin correlation, through a mechanism suggested by a recent impurity model study [6]. Implications of our results for the physics of iron-based superconductors and coupled flat-wide band systems are discussed.

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