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Local Moment Formation of an Anderson Impurity on Graphene
CHUNHUA LI, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas, 77204, USA, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, C. S. TING, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas, 77204, USA — We study the effect of a magnetic impurity on a single layer of graphene within an Anderson impurity model. Due to the vanishing local density of state at the Fermi level in graphene, the impurity spin cannot be effectively screened out. Treating the problem within the Gutzwiller approximation, we found a region in the parameter space of U-E^f where the impurity electron is in the local moment state, which is characterized by a zero effective hybridization between the bath electron and magnetic impurity. Here U is the onsite Coulomb repulsion of the impurity and E^f is its energy level with respect to the Fermi energy. The competition between U and E^f is also discussed. While larger U reduces double occupation and favors local moment formation, a deeper impurity level prefers double occupation and a nonzero hybridization and thus a Kondo screened state. For a fixed U, by continuously lowering the impurity level, the impurity first enters from a Kondo screened state to a local moment state and then departs from this state and re-enters into the Kondo screened state.

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