Vacancy-induced tunable Kondo effect in twisted bilayer graphene

Yueqing Chang[1, 2, *], Jinjing Yi[1, 2], Ang-Kun Wu[1, 2], Fabian B. Kugler[3, 1, 2],
Eva Y. Andrei[1], David Vanderbilt[1, 2], Gabriel Kotliar[1, 2, 4], and J. H. Pixley[1, 2, 3, †]
[1]*Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854, USA*
[2]*Center for Materials Theory, Rutgers University, Piscataway, NJ 08854, USA*
[3]*Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010, USA*
[4]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11973, USA*

In single sheets of graphene, vacancy-induced states have been shown to host an effective spin-1/2 hole that can be Kondo-screened at low temperatures. Here, we show how these vacancy-induced impurity states survive in twisted bilayer graphene (TBG), which thus provides a tunable system to probe the critical destruction of the Kondo effect in pseudogap hosts. Ab-initio calculations and atomic-scale modeling are used to determine the nature of the vacancy states in the vicinity of the magic angle in TBG, demonstrating that the vacancy can be treated as a quantum impurity. Utilizing this insight, we construct an Anderson impurity model with a TBG host that we solve using the numerical renormalization group combined with the kernel polynomial method. We determine the phase diagram of the model and show how there is a strict dichotomy between vacancies in the AA/BB versus AB/BA tunneling regions. In AB/BA vacancies, we find that the Kondo temperature at the magic angle develops a broad distribution with a tail to vanishing temperatures due to multifractal wavefunctions at the magic angle. We argue that the scanning tunneling microscopy response in the vicinity of the vacancy can act as a non-trivial probe of both the critical single-particle states and the underlying many-body ground state in magic-angle TBG.

--
[*]yueqing.chang@rutgers.edu
[†]jed.pixley@physics.rutgers.edu

Reference: arXiv:2312.09286