A unified theory of quasiparticle interference from defects in two-dimensional materials

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Abstract

Quasiparticle interference (QPI) measured by low-temperature scanning tunneling spectroscopy (STS) accompanied by a Fourier transform analysis (FT-STS) provides unique insight into defect-induced carrier scattering inside and between valleys in two-dimensional (2D) materials. Here I present a general T-matrix based framework for the calculation of FT-STS spectra which, in combination with atomistic DFT calculations of the defect scattering potential, allows for detailed modeling of FT-STS spectra for "realistic" defects such as, e.g., atomic vacancies, adatoms and substitutional atoms [1, 2].

In monolayer transition metal dichalcogenides (TDMs; MX2), atomic vacancies are commonly believed to be a source of pronounced intervalley scattering, thereby presenting a serious obstacle for applications exploiting their unique valley-contrasting properties. However, as I here show, the symmetry of the defect site gives rise to selection rules which protects against intervalley scattering. In the conduction-band FT-STS spectra this manifests itself by a K ↔ K' intervalley peak which is missing for X vacancies, while appearing clearly for M vacancies. These findings put the recent observations of absent K ↔ K' intervalley peaks in QPI experiments [3, 4] in a new perspective.

In graphene, the chiral nature of the states leaves clear fingerprints in the FT-STS spectra [5, 6]. For example, the central q=2kF backscattering ring around at the Γ point is strongly suppressed when trigonal warping is small -- this in spite of the fact that atomic defects often break the A,B sublattice symmetry thus allowing for backscattering. The reason for this apparent paradox as well as the reappearance of the backscattering ring at the Bragg points [5,6] emerges straightforwardly from our unified theory. As I furthermore demonstrate, resonant scattering due to defect-induced localized states on the Dirac cone strongly modifies this picture by introducing a hitherto unexplored variant of the backscattering ring at the center of the Brillouin zone.

References