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) companied 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; MX_2), 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 $K \leftrightarrow K'$ intervalley peak which is missing for X vacancies, while appearing clearly for M vacancies. These findings put the recent observations of absent $K \leftrightarrow K'$ 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 $q=2k_F$ 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 straight forwardly 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

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