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Interpretation of scanning tunneling quasiparticle interference and impurity states¹ ANDREAS KREISEL, Niels Bohr Institute, Denmark, P. CHOUBEY, University of Florida, USA, T. BERLIJN, Oak Ridge National Laboratory, USA, B.M. ANDERSEN, Niels Bohr Institute, Denmark, P.J. HIRSCHFELD, University of Florida, USA — We use a simple method of calculating inhomogeneous, atomic-scale phenomena in superconductors to obtain real-space conductance maps as measured in scanning tunneling spectroscopy (STM). Our approach makes use of first principles Wannier functions in conjunction with self-consistent solutions of the Bogoliubov-de Gennes equations on a lattice to image superconducting phenomena[1]. This method is a powerful tool since it captures correctly local symmetries on the surface that can be lower than the global lattice symmetry; it improves the spatial resolution from one pixel per lattice point to the sub-atomic scale; and simplifies the interpretation of STM data. As an example, we show how the pattern observed around a Zn impurity in BSCCO-2212, can be understood by accounting for the tails of the Cu Wannier functions^[2], and thus compare perfectly to experimental findings. Further applications of this method include the investigation of impurity states in multiorbital systems as well as the study of quasi particle interference phenomena to enable a better understanding of novel phenomena in high temperature superconductors. [1] Choubey, et al., Phys. Rev. B 90, 134520 (2014) [2] Kreisel, et al., arxiv.org:1407.1846 (2014)

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