Towards large-scale conductance simulations of twisted bilayer graphene: the CAP-Chebyshev method

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Realistic conductance simulations of real space twisted bilayer graphene (TBG) devices remains a demanding task. Specifically, the impact of moiré supercells on charge carrier transport requires giant system sizes to be considered. Near the magic angle, a single supercell reaches a size of about 15nm; ~10^4 cells are often needed to reach the experimentally relevant diffusive regime. Here, we develop a large-scale linear-response simulation ("CAP-Chebyshev") framework, combining Chebyshev approximation theory with a complex absorbing potential (CAP), to efficiently account for semi-infinite contacts [1-4]. Our method is benchmarked in a large 2-terminal 100nm x 100nm TBG model system containing 2.3×10^6 atomic orbitals. Exactly at the magic angle 1.24° , the conductance exhibits a peak at the charge neutrality point [Fig. 1] - evidence of a strong interlayer coupling state and a flat band supermetallic phase [5]. Finally, our framework is used to investigate the impact of twist-angle disorder on a 50nm x 50nm magic angle TBG device.

References

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Figures

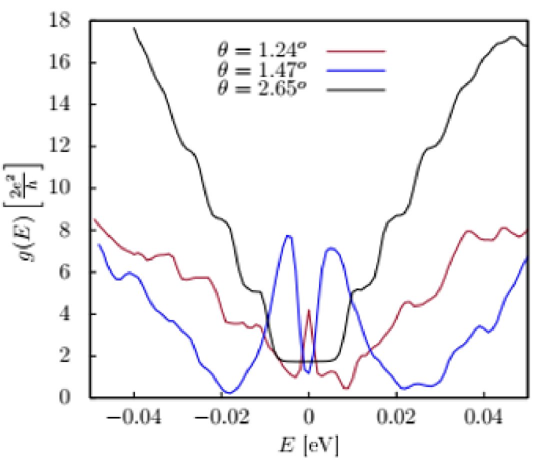

Figure 1: Conductance of the 100nm x 100nm TBG device as a function of the Fermi energy for different twist angles.