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Characterizing Destructive Interference Features in Molecular Transport Junctions[1] PANU SAM-ANG, MATTHEW REUTER, Department of Applied Mathematics and Statistics and Institute for Advanced Computational Science, Stony Brook University — Destructive interference features in molecular electron transport have recently attracted a lot of interest due to their unconventional behavior in electronic devices. Previous analyses have developed guidelines for predicting the existence and locations of interference features, but are limited to particular classes of molecules. In this work, we build on these results to understand interference features in terms of molecular orbitals, thereby developing physical intuition for the interference features. We also provide an analysis for characterizing destructive interference features; for example, their locations and robustness. Our methodology is more general than previous analyses because it applies to a broader class of molecules than conjugated hydrocarbons, and it has the additional benefit of working with the molecular Hamiltonian (as opposed to the Greens function). We illustrate the analysis with several molecules, including benzene, derivatives of anthraquinone, and cross-conjugated molecules.

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