

Abstract Submitted
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Exorcising Ghost Transmission from Electron Transport Calculations: Refighting Old Battles in New Contexts MATTHEW REUTER, Northwestern University, ROBERT HARRISON, Stony Brook University — First-principles calculations of electron transport aim to understand the dynamics of electrons as they traverse quantum mechanical systems. For instance, how does electric current travel through a molecule? Despite their successes over the years, these calculations are known to be haunted by several numerical artifacts. Ghost transmission is among the most serious of these unphysical results, causing transmission coefficients to show an extreme dependence on the basis set and to be many orders of magnitude too large. In this talk, we discuss electron transport formalisms, uncover the cause of ghost transmission, develop exorcism strategies, and present several numerical examples. In the end, ghost transmission is a ramification of poorly chosen spatial partitions. Instead of choosing partitions with the basis set (in a manner reminiscent of Mulliken or Löwdin population analyses), the relevant projection operators must be selected without referencing the basis set.

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