

Abstract Submitted
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A Physical Interpretation of an Orthogonal Hilbert-Space Transformation: Transmission Antiresonances from Long-Range Hopping SETH RITTENHOUSE, Dept. of Physics/Astronomy, Western Washington University, BRAD JOHNSON, Dept. of Physics/Astronomy, Western Washington University — We provide the physical interpretation for a recently- introduced Hilbert space transformation from a nonorthogonal (overlapping) basis to an orthogonal basis, for the purpose of studying transport through single-molecule systems. The new Hilbert space may be interpreted as an orthogonal basis in the same *physical* space, wherein the basis overlap is formally transferred to the hopping matrix elements in the orthogonal system, resulting in a standard tight-binding system in an orthogonal basis with long-range hopping. We utilize the formal procedure to solve for the transmission characteristics of an impurity site (molecule) coupled with semi-infinite leads. We demonstrate that (previously predicted) transmission antiresonances are produced, in the orthogonal space, by the presence of second-nearest neighbor hopping. The parameter range in which transmission antiresonances are possible is formally outlined—a feature of the orthogonal space transformation.

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