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Deciphering the Landauer-Büttiker Transmission Function from Single Molecule Break Junction Experiments MATTHEW REUTER, Department of Applied Mathematics and Statistics and Institute for Advanced Computational Science, Stony Brook University, STEPHEN TSCHUDI, Stony Brook University — When investigating the electrical response properties of molecules, experiments often measure conductance whereas computation predicts transmission probabilities. Although the Landauer-Büttiker theory relates the two in the limit of coherent scattering through the molecule, a direct comparison between experiment and computation can still be difficult. Experimental data (specifically that from break junctions) is statistical and computational results are deterministic. Many studies compare the most probable experimental conductance with computation, but such an analysis discards almost all of the experimental statistics. In this work we develop tools to decipher the Landauer-Büttiker transmission function directly from experimental statistics and then apply them to enable a fairer comparison between experimental and computational results.

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