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Many-body theory of electron transport in single-molecule junctions CHARLES STAFFORD, JUSTIN BERGFIELD, University of Arizona — Currently, there is no general theory to treat the many-body problem of a single molecule coupled to metallic electrodes. Mean-field approaches such as density-functional theory—the dominant paradigm in quantum chemistry—have serious shortcomings because they do not account for important interaction effects like Coulomb blockade. We develop a systematic theoretical framework for this nonequilibrium many-body problem, starting from an exact diagonalization of the few-body problem of an isolated molecule, and including lead-molecule coupling perturbatively in a novel application of nonequilibrium Green's functions.

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