Nonequilibrium diagrammatic technique for Hubbard Green functions¹ FENG CHEN, Department of Physics, University of California, San Diego, La Jolla, CA 92093, MAICOL OCHOA², MICHAEL GALPERIN, Department of Chemistry and Biochemistry, University of California, San Diego, CA 92093 — Utilizing many-body states of the isolated molecule, Hubbard nonequilibrium Green function (NEGF) is able to account for the intra-system interactions exactly while coupling to the contacts is treated perturbatively. We introduce nonequilibrium diagrammatic technique for the Hubbard NEGF, which allows building controlled approximations for both Green (two-time) and multi-time correlation functions. The formulation is an extension of equilibrium considerations for strongly correlated lattice models to nonequilibrium realm of current carrying molecular junctions. We demonstrate viability of the approach with numerical simulations for a generic junction model of quantum dot coupled to two electron reservoirs.

¹US Department of Energy under DE-SC0006422 and the National Science Foundation under CHE - 1565939
²Present Address: Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA

Feng Chen
Department of Physics, University of California, San Diego, La Jolla, CA 92093

Date submitted: 21 Sep 2016

Electronic form version 1.4