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Electron correlations in molecular wires: e-e interactionion both in leads and bridge[1] YURI DAHNOVSKY, Department of Physics & Astronomy, University of Wyoming, Laramie, WY 82071, VINCE ORTIZ, Department of Chemistry & Biochemistry, Auburn University, Auburn — Molecular systems (molecules) with strong electron-electron interaction both in leads and a bridge are described in terms of the time-dependent electron Green functions. We prove that the Meir-Wingreen expression holds if one assumes that the bridge and lead electron subsystems are strongly separated. We develop a diagrammatic technique in a well determined, noncrossing cluster approximation. Within this approach, Dyson equations for various nonequilibrium Green functions are derived, and the validity conditions are found. In addition, we rigorously prove that despite strong electron-electron or electron-viration interaction in the systems with the finite number of quantum states, the Landauer-Buttiker expression for electric current is true. The ab initio electron propagator method is applied to the calculations of I-V characteristics in molecular electronic devices with the bridge composed from 1,4–benzene–dithiolate molecule.

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