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Is a molecule a quantum wire or a quantum dot? BHASKARAN MURALIDHARAN, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, AVIK W. GHOSH, Dept. of Electrical and Computer Engineering, University of Virginia, Charlottesvile, VA 22904 , SUPRIYO DATTA, School of Electrical and Computer Enginnering, Purdue University, West Lafayette, IN 47907 — We address an important issue regarding the appropriate transport regime for molecular conduction. A typical transport calculation employs the Non Equilibrium Green's function (NEGF) transport scheme coupled with an appropriate self consistent field (SCF) method. This implies that the molecule is treated as a "quantum wire", usually applicable when contact couplings are much larger than other energy scales involved. However, there exists a whole class of experimental data whose qualitative features depart significantly from the ones usually explained using the above approach. We show that these features can be naturally addressed by adopting a Coulomb Blockade (CB) approach used in "quantum dot" transport. This involves description of the molecule in its many-body space. Our analysis in the many-body space of a prototypical molecule explains the non-trivial features commonly observed in low temperature molecular conduction experiments. Hence, we point out the inadequacy of SCF approaches towards a concrete description of molecular conduction which should involve both quantum chemistry and transport in the many-body space of the molecule.

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