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**Comparison of transport calculations using complex absorbing potentials and the Non-equilibrium Green's function formalism** KALMAN VARGA, JOSEPH DRISCOLL, Vanderbilt University, Nashville — In the Non-equilibrium Green's formalism (NEGF) the system is divided into left and right leads and a central region. To avoid spurious reflections from the boundaries one has to treat the leads as semi-infinite systems. Various efficient recursion methods are developed [1] for this purpose. Alternatively, one can use a complex absorbing potential (CAP) that absorbs the outgoing waves and one only has to deal with short finite leads. In this work we have compared the NEGF recursion and CAP approaches (1) on a simple analytically solvable example and (2) by calculating the transmission coefficients for a carbon nanotube device using a density functional Hamiltonian. Both approaches give very accurate results but the CAP method is orders of magnitude faster in calculating the self-energies. This work was supported by NSF grant ECS 0622146.

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