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Quantum transport in molecular electronic devices described with complex source and sink potentials[1] FRANCOIS GOYER, ALI GOKER, MATTHIAS ERNZERHOF, Universite de Montreal, UNIVERSITE DE MONTREAL TEAM — We present a non-Hermitian model Hamiltonian containing complex potentials [1,2] that is devised to study ballistic transport in molecular electronic devices (MEDs). The complex potentials replace semi-infinite contacts and act as source and sink of probability current density. This approach is rigorous in the sense that the exact wave function is recovered in the interior of the MED. We employ this technique to calculate the conductance through certain prototypical MEDs [3]. We also extend this method [4] such that we can go beyond the one- electron picture by constructing two-electron states explicitly. We present results for simple model system described by Hubbard-type Hamiltonians. The impact of electron correlation effects on the molecular conductance is discussed. [1] F. Goyer, M. Ernzerhof, M. Zhuang, JCP, 126, 144104 (2007). [2] M. Ernzerhof, JCP, to appear nov. 2007. [3] M. Ernzerhof, H. Bahmann, F. Goyer, M. Zhuang, P. Rocheleau, J. Chem. Theory Comput., 2, 1291 (2006); M. Ernzerhof, M. Zhuang, P. Rocheleau, JCP, 123, 134704 (2005). [4] A. Goker, F. Goyer, M. Ernzerhof, work in pogress.

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Ali Goker
Universite de Montreal

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