Extension of the Source-Sink Potential (SSP) approach for multiple channels conductance calculations

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In molecular electronics, molecules are connected to macroscopic contacts and the current passing through is studied as a function of the applied voltage. We focus on modeling the transmission of electrons through such a molecular electronic device (MED). Based on a simple Hückel Hamiltonian to describe the π electrons in conjugated systems, the SSP method [1] employs complex potentials to replace the wavefunction of the infinite contacts in a rigorous way. This method takes advantage of the known asymptotic form of the wavefunction in the contacts and yields a simple expression for the electron transmission probability [2,3]. The initial SSP approach [4] was limited to two one-dimensional contacts, here we extend the approach to multiple channels, i.e., to two-dimensional contacts including transverse modes. We describe the development of the method and illustrate it with applications.

References:

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