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Transport in closed nanoscale systems NEIL BUSHONG, NA SAI, MASSIMILIANO DI VENTRA, University of California, San Diego — An alternative way to describe electrical transport in nanoscale systems has been recently proposed where two large but finite charged electrodes discharge across a nanoscale junction (M. Di Ventra and T. Todorov, J. Phys. Cond. Matt. 16, 8025 (2004)). We have applied this concept to describe the dynamics of a finite quasi-one dimensional gold wire using both a simple tight-binding model and time-dependent density-functional theory. After an initial transient, a quasi-steady state sets in whose lifetime increases with system size. This quasi-steady state is due to the wave properties of the electron wavefunctions and the resultant uncertainty principle and is established without inelastic effects. The corresponding current-voltage characteristics at steady state are in very good agreement with those calculated from the static scattering approach. We discuss local electron distributions, electrostatic potentials, and local resistivity dipoles formed at the quasi-steady state and compare these findings with the static open-boundary problem. A relation between information entropy and electron dynamics is discussed. Work supported by NSF.

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