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Classical Nuclear Motion in Quantum Transport[1] CLAUDIO VERDOZZI, GIANLUCA STEFANUCCI[2], CARL-OLOF ALMBLADH, Department of Physics, Lund University, Lund, Sweden — A quantum-classical scheme is presented to study nuclear motion in time-dependent quantum transport. The nuclei are treated in the Ehrenfest approximation. We illustrate the method in terms of model systems results. We show how electron-lattice interactions may induce dynamical Peierls distortions in short wires, and change their conducting behavior. We also show time-resolved results for current-induced molecular desorption and suggest that AC biases could provide a way to tailor electromigration. The results illustrate the importance of non-adiabatic effects for transient phenomena in nanodevices.

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