Classical Nuclear Motion in Quantum Transport\textsuperscript{1} CLAUDIO VERDOZZI, GIANLUCA STEFANUCI\textsuperscript{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.

\textsuperscript{1}Work supported by the European Community 6th framework Network of Excellence NANOQUANTA (NMP4-CT-2004-500198)

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