Interplay of current-induced forces and electronic friction in nanoscale junctions far from equilibrium

E.K.U. Gross

Tsientang Institute for Advanced Study, Quantum Dynamics Laboratory, 181 Geyazhuang, Hangzhou, China

Nano-scale junctions consisting of a single molecule or a quantum dot sandwiched between macroscopic metallic leads show a rich variety of non-equilibrium phenomena when exposed to a sufficiently large bias. For example, Coulomb blockade manifests itself in the time-domain as a periodic charging and discharging of the central quantum dot [1]. In this lecture, special attention will be paid to the current-induced forces on the nuclei. The real-time dynamics of the system is simulated by combining Ehrenfest dynamics with time-dependent density functional theory (TDDFT). Electronic viscosity is accounted for by the frequency-dependence of the TDDFT exchange-correlation kernel. To understand the subtle interplay between the current-induced forces on the nuclei and electronic friction, we study the translational, vibrational, and rotational motion of a diatomic molecule immersed in a current-carrying electron liquid [2]. Starting from the nuclear equilibrium distance and applying a current pulse, we first observe acceleration of the nuclei due to the initial dominance of the current-induced push. After this initial phase, stabilization sets in upon balancing of the two forces, and finally, deceleration is caused by the friction after the end of the pulse. Based on these observations, we then explore the design of an atomic "waterwheel" [3], periodically driven by an AC current flowing in the electron liquid. A steady rotation of the molecule can be achieved for certain combinations of the amplitude and frequency of the imposed AC current. For other combinations, the nuclear motion turns out to be chaotic. The somewhat unusual forces appearing here will be analyzed in terms of the exact factorization. [4,5,6].

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