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Vibrationally Induced Decoherence in Single-Molecule Junctions: The Role of Electron-Hole Pair Creation Processes RAINER HARTLE, Department of Physics, Columbia University, MICHAEL BUTZIN, PEDRO B. COTO, Institut fur Theoretische Physik, Universitat Erlangen-Nurnberg, STEFAN BALLMANN, HEIKO B. WEBER, Lehrstuhl fur Angewandte Physik, Universitat Erlangen-Nurnberg, MICHAEL THOSS, Institut fur Theoretische Physik, Universitat Erlangen-Nurnberg — We investigate quantum interference effects and vibrationally induced decoherence in single-molecule junctions, employing nonequilibrium Green's function theory [1]. Molecular junctions often exhibit quasidegenerate electronic states that allow an electron to tunnel through the junction in different ways [2,3]. The respective outgoing wavefunctions interfere constructively or destructively, leading to an increase or decrease of the tunnel current, respectively. Interaction of the tunneling electrons with the vibrational degrees of freedom of the junction, however, gives 'which-path' information about the corresponding tunneling pathways because of the state-specific nature of electronic-vibrational coupling [2,3,4]. We demonstrate how this interplay between interference and vibrationally induced decoherence results in a strong temperature dependence of the current and highlight the role of electron-hole pair creation processes in this context [3,4]. To this end, we employ both generic models of single-molecule junctions as well as realistic models that are based on first-principles electronic structure calculations. [1] Phys. Rev. Lett. 102, 146801 (2009), [2] Phys. Rev. Lett. 107, 046802 (2011), [3] Phys. Rev. Lett. 109, 056801 (2012), [4] arXiv:1209.5619 (2012).

Rainer Hartle
Department of Physics, Columbia University

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