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Theoretical study of vibrational effects in molecular transistors

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Molecular devices raise the fundamental issue of non-equilibrium quantum mechanics of strongly correlated systems. This talk presents a complete theory of a model system (resonant level coupled to leads and a local oscillator) which captures an essential aspect of molecular devices and provides a context for strong correlation physics. The limits of high temperature (all coupling) and weak coupling (all temperatures) are treated by standard rate equation and Keldysh diagrammatic methods. Saddle point methods are developed for the more challenging low temperature strong coupling regime. The key issue is the formulation and solution of rate equations for the steady state reduced density matrix. Solutions of non-equilibrium mean field equations are shown to correspond to the field values at which the density matrix is peaked in a semiclassical limit. If multiple solutions exist, all are found to make non-vanishing contributions to physical quantities, implying absence of bistability in the current but structure in the noise. Departures from equilibrium produce decoherence that prevents the formation of characteristically quantal features such as the polaron peak in the spectral function. Generalizations of the method to other strongly correlated systems such as the non-equilibrium Kondo model will be given. Ref: Phys. Rev. B 69, 245302 (2004) and cond-mat/0409248. This work was performed in collaboration with Igor Aleiner and Andrew Millis and was supported primarily by the Nanoscale Science and Engineering Initiative of the National Science Foundation under NSF Award Number CHE-0117752 and by the New York State Office of Science, Technology, and Academic Research (NYSTAR).