Thermodynamics of strongly coupled driven quantum systems

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The driven resonance level model (a driven molecular level coupled to one or more fermionic baths) has been recently used to study thermodynamic aspects of energy conversion in simple mechanically driven strongly coupled quantum systems. Our original treatment of this problem was based on the non-equilibrium Green function (NEGF) approach [1]. In this talk I will discuss this model using other methodologies that reveal different physical aspects of this problem. First, I will describe an approach [2] based on an expansion of the full system-bath density matrix as a series in powers of the modulation rate, from which the functional form of work, heat, and entropy production rates can be obtained. This approach allows for the inclusion of electron-electron interaction in an approximate way. Second, I repeat the derivation by expressing the density matrix in terms of the asymptotic eigenstates of the system by employing Moller transition operators [3]. The resulting expression, which coincides with results from the steady-state theories of McLean – Zubarev and Hershfield, can reproduce the standard NEGF results for the dot population and the current and, when extended to include driving of the dot energy level and/or the dot-leads coupling, yields the non-adiabatic (second order to the driving speed) corrections to the power, energy and heat production obtained from the NEGF formalism. Using this approach we can easily go beyond the wide band approximation and consider models where the dot is coupled to many leads held at different temperatures and under different chemical potentials. Finally, we employ a numerical solution based on the driven-Liouville-von Neumann approach [4], which reproduces the results obtained from the analytical approaches for slow driving and can be used to investigate systems subjected to high driving speeds.

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