Numerically exact full counting statistics of the Anderson impurity model

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The full characterization of charge and energy transfer processes in molecular junctions requires techniques for evaluating higher-order statistical cumulants of the different transfer processes. The complete set of cumulants gives access to the full counting statistics (FCS) through the so-called cumulant generating function (CGF) [1].

Previously, the computation of the CGF for the evaluation of FCS in fermionic systems has been restricted to either noninteracting [2] systems or to specific limiting parameter ranges in correlated systems [3]. Despite the existence of various approximation methods, only very few numerically exact results exist in this field. In this talk, I present a new method [4] for calculating the FCS of a generic nonequilibrium interacting fermionic model, valid for arbitrary temperatures, voltages and interaction strengths. This method is based on the recently-developed inchworm diagrammatic quantum Monte Carlo (iQMC) method [5]. It will be discussed how, using a modified hybridization expansion [6] of the generating function for the FCS in the Anderson impurity model (AIM), the problem of FCS can be mapped to an equivalent problem in iQMC.

To test the method, we present noninteracting benchmarks against path integral techniques [2]. We then go on to discuss the effect of electron-electron interactions on time-dependent charge cumulants, the first passage time distribution (FPTD) and probability distributions for the transfer of n-electrons, as well as the heat current and associated noise. We find 'queuing' behaviour in the FPTD caused by electronic correlations, and discuss how this is manifested in the n-particle probability distribution functions. We observe a fascinating crossover in the shot noise from Coulomb blockade to Kondo effect – dominated physics. Finally, we show how the quantum master equation (QME) approach to FCS fails to capture finite bandwidth effects in the current-voltage and noise-voltage characteristics of the AIM [7].

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