Report on “Noise and Full Counting Statistics of electronic transport through interacting nanosystems”

The report addresses the topic of full counting statistics (FCS) in electron transport through nanoscale systems. When considering the modeling of current flow across nanoscale junctions, the central quantity is the probability distribution that a certain number of electrons have travelled through the system at a given time. Encoded in the distribution function are the electronic properties of thw system and the transport mechanisms at play. Analysis of the different quantities derived from distribution function can thus provide insight into the behavior of the nanoscopic system and FCS focuses on the cumulants of the distribution.

Concerning electron flow, the most obvious quantity that can be calculated (or measured) is the current. This is the first cumulant of the distribution, the average number of electrons passing through the system gives the current, which is the quantity most commonly measured in experiments. Shot noise, the noise when large voltages are applied, can also be measured in experiments and is proportional to the second cumulant. Analysis of these and higher-order cumulants thus provides useful information on the mechanisms of electron transport.

The report starts by briefly introducing the essentials of full counting statistics and key concepts in a clear way.

The second chapter illustrates classical counting statistics by considering the case of a single electronic level. Here, spin degrees of freedom are not important and just result in a factor 2 in the calculated current. This single electronic level is weakly coupled to the leads: its value is small compared to other relevant energy scales such as the position of this level with respect to the chemical potential of the electrodes, or with respect to the temperature kT. The dynamics of electron transport can be described with a master equation for a probability distribution function giving the occupation of the level (empty, occupied) and a given number of charges having been transferred across the level. The cumulants of the distribution can be obtained analytically.

Of particular interest are two limits. The first one is the equilibrium case (zero applied) voltage. Here, the electric current is zero however, there are of course fluctuations coming from the stochastic nature of the electron transport process. In this limit, the cumulant generating function contains higher order terms in the counting field and is not simply a quadratic function. Therefore, even at equilibrium, thermal fluctuations in the current contain contributions of higher order cumulants and is not merely quadratic. The other limit of interest is that of high applied voltages. This is the shot noise limit. The current and noise can be expressed analytically in terms of the Fano factor, which tends to the value ½ for a symmetric junction and to 1 for a strongly asymmetric junction. In the latter case, the transport processes is limited by the contact with the smaller coupling and the counting statistics are well described by the Poissonian limit.

The last part of chapter 2 deals with the effect of vibrations on the transport characteristics of a single level model in the limit of large voltages. This is an interesting addition since it discusses a prediction on the dependence of the cumulants with voltage that is contrasted with another one in the literature. In this voltage limit, vibrations are slow compared to the timescale for the electron to be transmitted through the system and the vibrations can then be considered to gate the electronic level. In a subsequent publication, these results were extended to account for energy exchange between tunneling electrons and the oscillator describing the vibrations. From a master equation for the joint probability density of oscillator occupation and transmitted charge, the cumulant generating function can be obtained. This result is interesting because if can be compared with one in the literature calculated from a fully microscopic model. This work in the literature predicts a dependence of the k-th current cumulant on the voltage that goes with the k+1 –th exponent. However, in the model described here the exponent is 2k. Experiments on high-order cumulants are not straightforward, however measurements should be able to resolve this discrepancy. P18, for example, points to relevant experiments and discusses the possible experimental verification. To attest to the importance and timelessness of the topic and of these contributions, this debate has had an impact in the field, having picked up by other researchers in the field (eg. in a 2016 publication by Prof. Segal).

The next chapter addresses nano-electro-mechanical systems (NEMS) and describes them typically using a generalized master equation approach. This is considered in the wide-band limit (where the energy dependence of the coupling to the leads is small and thus ignored), and under a large applied voltage where one of the leads is occupied while the other empty. This approach is quasi-classical, where the electron hopping is instantaneous and classical, while the description of the system (dot and/or leads) is done at the quantum level. This has led to the term “quantum shuttle” for typical NEMS. A probability distribution for the density operator, determined from the generalized master equation, allows for the calculation of the cumulants. This is not straightforward and numerical methods developed to tackle this are mentioned. Markovian generalized master equations are also mentioned, and the author’s contributions described well. Other numerical methods, such as Quantum Monte Carlo techniques, are also mentioned. The discussion of these methods serves to illustrate the current timely topics in the field and the author’s contributions. The third chapter ends by illustrating how full counting statistics can discriminate between the different transport mechanisms under consideration. The authors had considered a quantum shuttle and had come up with two plausible transport mechanisms: tunneling (where the dot s stationary) and shuttling (where it oscillated back and forth). In a later paper, they conjectured that there was the bistable coexistence of these two mechanisms with long timescales. The switching rates between the mechanisms was extracted from the first cumulants, and then substituting them in the equation for the third cumulant. The expression for the third cumulant thus obtains was compared to a fully numerical solution. The agreement between both approaches validates the approach and, importantly, illustrates clearly the role of full counting statistics in discerning different electron transport mechanisms.

Chapter 4 studies counting statistics in the fully quantum regime, where coherence effects are essential. As stated, this is intimately related to measurements of quantum systems. If the measurement probe is introduced far from the coherent region, this makes the measurement essentially classical. If, on the other hand, the probe is embedded in the region where coherence is important, then the probe itself must be included in the quantum-mechanical treatment. The formula for the cumulant generating function in the quantum regime is presented on the Keldysh contour. The system Hamiltonian can be modified through a gauge transformation. The cumulants are obtained from derivatives of the cumulant generating function for large times with the appropriate ordering of operators in the contour.

This approach can also be used to compute the reduced density matrix from modifications of the Liouville – von Neumann equation for the density matrix of the whole system. A method for evaluating high-order cumulants in non-Markovian generalized master equations is discussed. The method is based on the perturbative expansion of extremal eigenvalue of the generalized memory kernel. For a single resonant level in the regime of Fermi edge singularity, an interaction term is added to the Hamiltonian to model the scattering of incident electrons in one of the leads by the occupied level. The corresponding interaction term for scattering in the other lead does not seem to play a role in relevant experiments. Under the appropriate applied bias, the resonant level matches the position of one of the chemical potentials of the electrodes and it is possible to integrate out the other electrode and apply a perturbative expansion in the lowest order in the coupling to the (remaining) lead. Under these conditions, a memory kernel is derived in terms of counting fields and (non-Markovian) tunneling rates. The mean current and noise cumulants are then obtained in terms of the Fano factor. The limiting expressions of these cumulants are shown in the shot noise limit and low enough temperature. The mean current and Fano factor as a function of the energy difference to the resonant edge shows strong differences as a function of temperature (around a temperature comparable to broadening due to tunneling). This behavior is discussed in terms of quantum-induced memory effects that are wiped out with increasing temperature.

The final section in the chapter describes an approach alternative to the generalized master equations for the determination of full counting statistics. The approach is based on Non-Equilibrium Green's Functions, a scheme also commonly used in electron transport theory. The counting field is introduced in the Hamiltonian, which is modified according to the part of the Keldysh contour. The cumulant generating function can be obtained from the Hamiltonian modified in this way, although the derivative of the adiabatic potential is the most useful quantity. This is an equal-time Green's function which involves the resonant level and leads. The case of a single resonant level with many-body interaction (localized to the level and not extending to the leads) is discussed. Compared to the situation where there are no counting fields, there are now some differences in the components of the Green's function, in particular all four Green's functions need to be retained in the perturbation scheme, but otherwise the formalism can be retained. The formalism reduces to the known Meir-Wingreen expression when the counting field is removed. The counting field is included in the Green's function, which also incorporates any many-body effects. Thus the evaluation of the Green's function is the central problem. This can be done via the Dyson equation. Several papers are discussed dealing with corrections to electron transport arising from inelastic effects. The electronic system is coupled to a single vibrational mode (one electronic level at first, in subsequent papers it was extended to a multilevel system). Interaction between electrons and vibrations was included at the second order in electron-vibration coupling. This perturbative treatment is usually sufficient. The quantity of interest here was the inelastic noise signal around the energy of the vibrational mode. The condition that the vibrational energy be much larger than the temperature is easily fulfilled in molecular junctions. The inelastic noise, obtained as a function of elastic transmission, can be either positive or negative, depending on the value of transmission itself. Generally it is positive (negative) when transmission is low (high). Comparison is made with experiments on Au atomic wires. Although the agreement is good, the predicted value of the crossover does not match experiments exactly, and the reasons for this are not yet clear. Nevertheless, further (challenging) experiments should significantly contribute to resolve this discrepancy.

In summary, the work summarized here represents significant contributions to the field of full counting statistics in interacting nanosystems. These results have addressed relevant and timely problems and have contributed important results. The corresponding papers are well known and well cited. Personally I value positively that, even though the nature of the work has been obviously theoretical, comparison with experiment has not been forgotten. Indeed, comparisons with measured results have been made or attempted, and predictions stand waiting experimental verification. Altogether I judge the significance of this work to be very high.

[redacted]

Héctor Vázquez