Transport through nanostructures: Finite time vs. finite size

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Numerical simulations and experiments on nanostructures out of equilibrium usually exhibit strong finite size and finite measuring time t_m effects. We discuss how these affect the determination of the full counting statistics for a general quantum impurity problem. We find that, while there are many methods available to improve upon finite-size effects, any real-time simulation or experiment will still be subject to finite-time effects: In short size matters, but time is limiting. We show that the leading correction to the cumulant generating function (CGF) at zero temperature for single-channel quantum impurity problems is proportional to $\ln t_m$, where the constant of proportionality is universally related to the steady state CGF itself for non-interacting systems; universal in this context means independent of details of the quench procedure, i.e., independent of the switching on of both voltage and counting field. We give detailed numerical evidence for the case of the self-dual interacting resonant level model that this relation survives the addition of interactions. This allows the extrapolation of finite measuring time in our numerics to the long-time limit, in excellent agreement with Bethe-ansatz results.

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Finite measuring time effects play a crucial role in the analysis of out-of-equilibrium properties of nanostructures [1]. This is clear in numerical simulations where, rather than solve an equilibrium eigenvalue problem, one time evolves from the nonequilibrium initial condition:

$$|\Psi(t)\rangle = e^{-i\hbar\mathcal{H}(t-t_0)}|\Psi(t_0)\rangle. \tag{1}$$

Time evolving a many-body state is a computationally expensive procedure, which gives a limit on the time scales accessible. The same is true of experiments, where one cannot measure the system for eternity. Indeed in recent experiments concentrating on the full counting statistics (FCS) [2–4], the source-drain bias voltage V_{SD} is so low that the relevant parameter $V_{SD}t_m$ is actually rather small.

Finite-time effects are often combined with finite-size effects, which are ever present for systems on nanoscale structures. In equilibrium, finite-size scaling is well under control, and often turns out to encode fundamental properties of the bulk system, for example, the relation between the $1/L$ (L being the system size) corrections to the ground state energy density and the central charge of the system [5,6]. The crucial point here is the *universality* of this relationship, meaning that details of the edge (such as precise boundary conditions) are unimportant.

By analogy, one may ask the following questions: Can one extrapolate short measuring time t_m results to the long-time limit? Is there any universality in these finite t_m corrections, and if so, can these corrections give us new information about the system? In this Rapid Communication, we will show that in certain situations the answer to all three of these questions in the case of the FCS is yes. This will require us to also disentangle the contributions that come from *finite size* and *finite time*.

The systems we consider are quantum impurities coupled to two noninteracting leads which are (initially) held at different chemical potentials. The finite size in question, L, is the size of the lead, the quantum impurity being naturally a small size. The plan for the rest of this Rapid Communication is to introduce the FCS, look at the intrinsically finite-size corrections, then turn to the major issue of the work: the intrinsically finite-time effects.

The transport properties of a nanostructure are not entirely encoded in the average current $\bar{I}$ flowing for a given bias voltage V_{SD}—fluctuations are of crucial importance, for example, in the determination of the charge of the carriers. The corresponding information is conveniently assimilated within the framework of FCS. In the traditional two-terminal setup, one studies the probability distribution $P_{t_m}(n)$ that a charge $Q = ne$ has been transferred from the left to the right lead in the measuring time t_m (e being the charge on the electron) [7–13]. Rather than working directly with the distribution, it is usually more informative to study the cumulant generating function (CGF), defined as [7,8]

$$F_{t_m}(\chi) = -\ln\left[\sum_n e^{in\chi} P_{t_m}(n)\right]. \tag{2}$$

The irreducible cumulants of charge transfer are then obtained via $C_n = -(\frac{\partial}{i\partial\chi})^n F(\chi)|_{\chi=0}$, while the periodicity of the CGF yields information regarding the charge of the quasiparticles involved in transport [10,14,15] which in a strongly correlated system may not be simple electrons, and may even undergo a change as a function of bias voltage [16,17]. In the long-time limit, each of the cumulants (and by inference, the CGF) is proportional to the measuring time t_m; for example, the first cumulant gives the current $C_1 \sim \bar{I}t_m$, while the second $C_2 \sim \bar{S}t_m$, where $\bar{S}$ is the zero-frequency shot noise.

In the present work, we will be interested in the leading corrections to these expressions for finite measurement times. However, we first discuss the corrections due to the finite size of the leads. To make this discussion concrete, we focus on the interacting resonant level model (IRLM), [17–26] described

by the Hamiltonian

$$\mathcal{H} = \sum_{n=L,R} \Bigg\{ -\sum_{i=0}^{M_n} (c^\dagger_{n,i} c_{n,i} + \text{H.c.}) + J' c^\dagger_{n,0} d + \text{H.c.} + U(d^\dagger d - 1/2)(c^\dagger_{n,0} c_{n,0} - 1/2) \Bigg\}. \quad (3)$$

Here, $d^\dagger$ creates a fermion on the resonant level, while $c^\dagger_{n,i}$ creates a fermion on the right or left lead at site i, the total size of each lead being $M_{L,R}$. The hybridization between the leads and the resonant level is J' (the hopping parameter on the leads which sets the overall energy scale of the problem has been set to 1), and U gives an interaction between the resonant level and the leads.

There are two values of U where the model has been solved out of equilibrium and transport properties are known: $U = 0$ is the noninteracting case [21–23], and $U = 2$ where the model shows a certain duality [17–20] although many works exist on the model at general U [24–26]. We imagine a situation where the two leads are initially decoupled from the resonant level, and exhibit a charge imbalance characterized by a difference in potential V_{SD}, modeling the source-drain potential in an experimental setup. At time $t = 0$, the coupling J' is quenched on, and a current begins to flow [27,28]; an extension of this method to calculate the CGF of FCS was recently expounded in [17]. We refer to the literature for a physical discussion of the transport properties of the RLM: Here we use it as a basis for discussions of the effects on transport of the finite size $M_{L,R}$ of the leads, and the finite measuring time t_{m} on the FCS. We expect our results to be applicable to more generic quantum impurity models.

One finds that there are three important consequences to having finite-size leads. The first concerns the discrete nature of the energy levels of the leads, leading to a finite-size energy gap, Δ. This means that all important physical processes must happen at energy scales larger than this gap. This is a phenomenon inherited from equilibrium problems, which remains relevant to the present nonequilibrium case. The second consequence also relates to the finite-size energy gap but is intrinsic to the transport—a coherent system with a gap exhibits oscillations in the dc transport. These were first observed in the current [19] but are also seen in all higher cumulants (or alternatively the CGF) [17]. Even in systems when the finite-size gap is unimportant for equilibrium properties, the oscillations $\sim\Delta\cos(V_{\text{SD}} t_{\text{m}} + \eta)$ may be clearly visible in nonequilibrium dc transport. These oscillations do not decay in time, and have the same physical origin as the Josephson effect, with the frequency given by the source-drain voltage V_{SD} and the amplitude proportional to the gap [19,28], i.e., proportional to $1/L$ if the leads are discretized uniformly in energy space. Furthermore, so long as one evolves in time for sufficiently long to see a few oscillations, results may be fitted using the above expression; this procedure has been remarkably successful provided the bias V_{SD} is not too small. The third consequence is that after a transit time $t_{\text{T}} = v_c L$ (where v_c is the excitation velocity in the leads) the excitations leaving one lead bounce off the edge of the other lead, which eventually causes the current to flow the other way. For details we refer to [28].

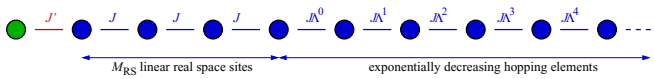

FIG. 1. (Color online) Setup of damped boundary conditions for a resonant level coupled to a single lead via a hybridization of J'. The lead first consists of a homogeneous tight binding chain (hybridization J), followed by exponentially decreasing hopping elements with a factor of Λ on each successive link in a NRG fashion. This increases the density of states at the Fermi surface.

In certain physical systems, including the (interacting) RLM, the finite-size gap is relatively harmless. However, in other systems epitomized by the Kondo effect, the emergent phenomena occur at low energy scales. In these cases Δ must be smaller than any physical scale in which one is interested. In equilibrium this problem may be solved via numerical renormalization [29,30]. One introduces a logarithmic discretization of the leads in energy space, which is transformed into a nearest-neighbor tight binding chain with exponentially decreasing hopping elements, leading to an exponentially enhanced density of states close to the Fermi surface. This approach has been extended to nonequilibrium systems [31] within a time-dependent NRG (td-NRG) method. Here, one solves the noninteracting scattering problem, discretizes the resulting scattering states in analogy to equilibrium NRG, and switches on interactions perturbatively. The concept of increasing energy resolution by changing the bond terms was extended to smooth boundary conditions [32] and to damped boundary conditions (DBC) in [33,34], where a homogeneous tight binding chain is inserted between the impurity and the exponentially damped region (see Fig. 1).

While this setup proved successful for the linear conductance of the IRLM [33] it is problematic for nonequilibrium properties. In [34] it was shown that in time-dependent simulations the exponentially decreased hopping elements lead to an exponentially decreased excitation velocity in the damped region, resulting in a NRG tsunami: The leads lose the property of a nicely behaved bath (see also [35]). Additionally, each link with changed hopping elements acts as an additional scatterer leading to an increased backscattering.

In Fig. 2 we show the current as a function of time following the charge imbalance quench for the noninteracting RLM with

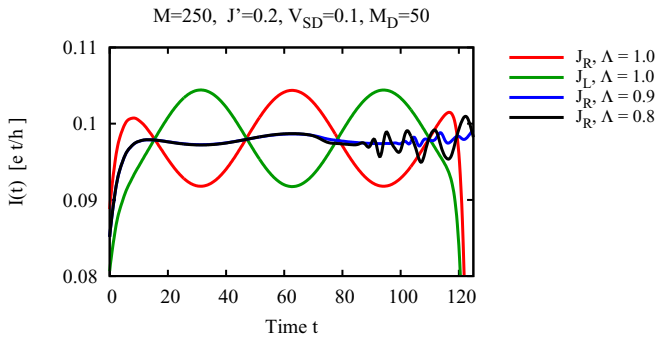

FIG. 2. (Color online) Time evolution of the current following a charge imbalance quench measured to the left (L) and right (R) of the resonant level in model (3) with $U = 0$ and $J' = 0.2$. The system size here is $M = 250$ sites, with DBC for various values of Λ in the setup shown in Fig. 1.

$J' = 0.2$ in a system with DBC, where the hopping elements on the last 50 sites of the left and right leads are decreasing with a factor of $\Lambda = 1.0$ (homogeneous leads), 0.9, and 0.8. The $\Lambda = 1$ displays the large Josephson oscillations (JO) as discussed above until the transit time t_T when we see the back reflection of the hard wall boundaries of the leads. It is worth noting that for this particular example though, there is a phase shift of π between the response left and right of the impurity; averaging over these dramatically decreases the size of the oscillations.

As one may expect, the DBC lead to a decreased height of the JO. However, the gain is not exponentially large, as we are now at finite voltage $V_{SD} = 0.1J$, while the DBC lead to exponentially enhanced density of states (DOS) at the Fermi surface only. One could use a different discretization scheme where the enhancement of the DOS is shifted to energies $\pm V_{SD}$ [34]. However one still faces the problem that each modified bond leads to a back reflection. The transit time for the DBC systems is decreased compared to the homogeneous case by $2M_D/v_c$, where M_D is the number of modified bonds. Accordingly, wiggles appear shortly after $t_T = (M - 2M_D)/v_c$. In principle, by using reflectionless DBC [36] one could avoid these wiggles, however, a reduced transit time remains.

We now turn to this issue of transit time, which places a hard limit on the time one may evolve the system before finite-size effects interfere with the time evolution. Here also, one can minimize this disruption (but only in a homogeneous lead) by using a *conformal time*. In equilibrium, it is well known how conformal invariance allows one, via a finite-size/temperature transformation, to control the effects of finite imaginary time [37]. The generalization to out-of-equilibrium situations and real time amounts to replacing the measuring time $t_m = t - t_0$ with the "conformal time"

$$d(t_m) = \left(\sin \frac{\pi t}{M/v_c} - \sin \frac{\pi t_0}{M/v_c} \right) \frac{M\pi}{v_c}, \tag{4}$$

where the counting field is switched on at $t = t_0$, after initially quenching the system at $t = 0$. While $d(t_m) \approx t_m$ at short times, as one approaches the transit time, the above formula captures the leading effects of back reflection from the leads remarkably well [38] (despite not being entirely justified theoretically [39]).

While this demonstrates an intimate connection between finite size and finite time, one may not always be able to time evolve the system as long as the transit time [40]. Furthermore, even if one manages to eliminate all finite-size effects, any real-time numerical simulation is cut off after some finite running time. We therefore turn to effects intrinsic to the finite measuring time of the system, studying the CGF of the FCS as a function of t_m.

As mentioned previously, one expects the CGF (2) to grow linearly in measuring time. At zero temperature, the subleading corrections are logarithmic [41,42],

$$\begin{aligned} F(\chi, t_m) &= \tilde{F}_0 t_m + \tilde{F}_1 \ln(V_{SD} t_m) + \cdots \\ \Rightarrow \dot{F}(\chi, t_m) &= \tilde{F}_0 + \tilde{F}_1/t_m + \cdots . \end{aligned} \tag{5}$$

Formally, this is an expansion of the CGF in the small parameter $(V_{SD} t_m)^{-1}$. The long measuring time limit $\tilde{F}_0$ is what is commonly quoted and analyzed as the FCS, and is given for noninteracting particles by the Levitov-Lesovik formula [7,8].

Here, we *conjecture* that the leading correction to this, $\tilde{F}_1$, is independent of the quench protocol (i.e., is a true steady state property), and given in the zero-temperature limit by

$$\tilde{F}_1 = \frac{1}{\pi} \left(\frac{d\tilde{F}_0}{dV_{SD}} \right)^2 . \tag{6}$$

Equation (6) is valid for single-channel quantum impurity problems, for systems symmetric with respect to the sign of the applied voltage. While it is only formally derived for noninteracting fermions, we will present arguments and numerical evidence that suggest it survives the addition of interactions. However we stress that a proof of this equation, or alternatively an understanding of the limits of its applicability, is an open question.

Equation (6) agrees with previously derived results for noninteracting fermions [1,41,42], where the only essential feature that goes into deriving this term is the Fermi-edge singularities [38]. Thus the result is limited to zero temperature, but does not involve details of the quench. For nonzero temperatures T, we would expect the result still to hold on time scales $t_m < 1/T$ [43]; at later times corrections to the long-time limit are no longer universal.

The fact that the physics of $\tilde{F}_1$ comes from the Fermi edge, which is explicitly captured by the derivative representation, Eq. (6), gives hope that this formula may also be valid in the interacting case. In a nearly-free-electron picture where interactions may be treated as perturbatively dressing free-electron results, one would certainly imagine that the relationship remains unchanged between $\tilde{F}_0$ which involves all states within an energy window of width V_{SD}, and $\tilde{F}_1$ which involves only the states at the Fermi edges. This can be made more formal by looking at the second cumulant (shot noise), where the correction according to Eq. (6) is $\propto G^2$, G being the differential conductance. The finite-time correction to the second cumulant of FCS is directly related to the finite-frequency correction to shot noise, something that has also been investigated in detail for the third cumulant [44]. This relation can therefore be compared to an earlier conjecture that the frequency-dependent noise $S(\omega) - S(0) \propto G^2|\omega|$. In [45], this was shown to be true to all orders in perturbation theory, while other work [46] suggested that this may break down in a nonperturbative regime. This question has been revisited recently numerically [20,21] which supported the idea that this simple relation holds even nonperturbatively.

While at present we are unable to give a more substantive analytic derivation of the conjecture (6), we now back it up with numerical evidence, using the self-dual interacting RLM. This is chosen as it exhibits nontrivial correlations, and is one of few such models where exact results for the FCS (in the long-time limit) are known analytically [17]. For convenience, the analytic results are given in the Supplemental Material [38]. In Fig. 3 we compare the real part of $\dot{F}$ obtained numerically with the analytic result including the $1/t_m$ correction, assuming that Eq. (6) holds. As can be seen there is nice agreement over four orders of magnitude. Although there appears a shift in each curve we mention that simulations are done on a lattice, while the analytic results are taken from a continuum theory

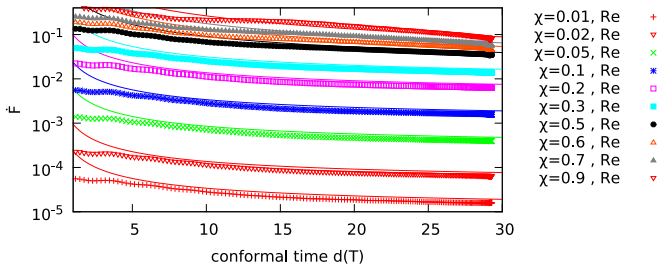

FIG. 3. (Color online) Real part of $\dot{F}$ for the SD IRLM at $V_{SD} = 0.3$, $J' = 0.2$. Symbols correspond to the numerical result, and the lines are the analytical results. The system size is $M = 240$ sites.

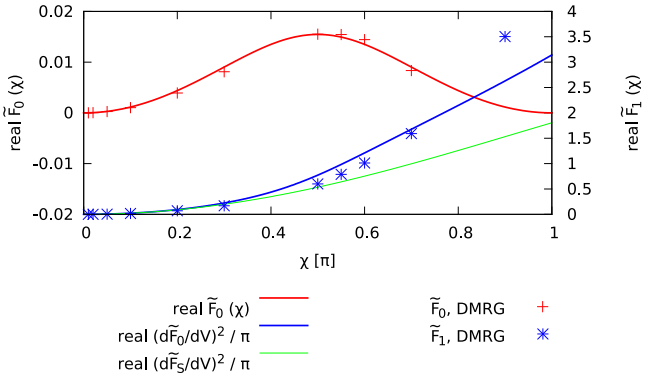

FIG. 4. (Color online) Comparison of the analytical and numerical results of the leading $\tilde{F}_0$ and subleading $\tilde{F}_1$ contributions to the CGF of the self-dual interacting RLM. The numerical results are obtained from fitting the real-time data in Fig. 3.

and the only scale parameter linking the two is taken from previous work [19]. Similar agreement is seen at other values of V_{SD} or J'.

Using these results we then perform a fit as a function of t_m to the series (5). To avoid influence of the transients, we limit the fit to $d(t_m) > 13$. These are compared to the analytic results in Fig. 4. One sees, in particular, very good agreement for $\tilde{F}_1$ until χ becomes too large, where the numerical data is very messy for reasons not yet fully understood. This gives excellent evidence in support of the conjecture (6). We also plot for comparison the quadratic in χ approximation to $\tilde{F}_1$, which is the correction to the shot noise (we note that the universal correction is absent for the first cumulant). It is clear from the plot that both the true $\tilde{F}_1$ from (6) and the numerical data deviate significantly from the quadratic approximation—in other words, we see beyond the lowest cumulants.

It is also worth noting the difference in scale for the $\tilde{F}_1$ and $\tilde{F}_0$ plots—the finite t_m correction is much larger than the long-time limit until $t_m \sim 100$. Nevertheless, a correct fitting procedure as a function of measurement time allows one to extrapolate over several orders of magnitude and see (to good agreement with the analytic result) the bump in the long-time CGF $\tilde{F}_0$; a feature that was entirely absent in the previous analysis [17].

In summary, we have discussed how dc transport calculations are subject to finite-time and finite-size effects which are of different nature. While finite-size effects can be controlled by a suitable choice of boundary conditions, the situation for finite-time effects is more difficult. By looking at the CGF one can perform a systematic extrapolation towards the long-time limit. In addition we showed that in the examples given the leading finite-time corrections are related to the long-time CGF itself [see Eq. (6)]. If such a relation holds more generally, it provides a fantastic possibility for self-consistency checks within time-dependent simulations. We therefore hope this Rapid Communication stimulates further work investigating a more general validity of (6).

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