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Reprint of : A computational approach to quantum noise in time-dependent nanoelectronic devices

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ABSTRACT

We derive simple expressions that relate the noise and correlation properties of a general time-dependent quantum conductor to the wave functions of the system. The formalism provides a practical route for numerical calculations of quantum noise in an externally driven system. We illustrate the approach with numerical calculations of the noise properties associated to a voltage pulse applied on a one-dimensional conductor. The methodology is however fully general and can be used for a large class of mesoscopic conductors.

1. Introduction

Among the many contributions of Markus Büttiker to the field of mesoscopic physics (now best known as nanoelectronics), his pioneer work on time-dependent phenomena was particularly dear to him. He insisted in pointing out the role of displacement currents (required to restore current conservation), the need for a theory that preserved "gauge invariance" and more generally built up the general framework and concepts to address this physics. While the key theoretical works were performed in the early 90s [1–5], the corresponding experiments were difficult (GHz physics at mK temperatures) so that more than 10 years elapsed before the first quantum RC circuit could actually be measured [6]. The field has considerably matured since then, with the latest generation of experiments performed directly in the time domain [7].

Markus visited Saclay on March 2006 which is when the senior author of this paper was introduced to the subject. At that time, although the analytical theory was well developed, its computational counterpart was still in its infancy (see [8] for a short history). We now have very effective numerical tools [8], with a computational effort linear both in time and system size, so that numerical complexity is no longer an issue [9] to simulate time-dependent systems. In this paper, we would like to extend these tools to calculate another quantity, also very dear to Markus, namely the quantum fluctuations of observables. Quantum noise is a quantity which is not only sensitive to the wave aspect of quantum transport but also to particle statistics [10]. We shall see that its numerical calculation requires some care in order to disentangle the relevant contributions from the large background already present at equilibrium.

2. The Pauli principle in driven mesoscopic systems

Let us consider a general mesoscopic system described by a time dependent (externally driven) quadratic Hamiltonian

$$\hat{\mathbf{H}}(t) = \sum_{i,j} \mathbf{H}_{ij}(t) c_i^\dagger c_j \tag{1}$$

where $c_i^\dagger$ (c_j) are the usual Fermionic creation (annihilation) operators of a one-particle state on site i. The site index i typically labels space as well as spin, orbital (s,p,d,f) and/or Nambu (for superconductors) degrees of freedom. The system is open, i.e. consists of a finite time-dependent central part connected to infinite (stationary) electrodes. We further suppose that the Hamiltonian is time independent for $t \leq 0$ and we switch on the time-dependent part (voltage pulses, light, etc.) at $t > 0$.

For $t \leq 0$, the solution to this problem is well known: one introduces the stationary scattering states $\Psi_{\alpha E}^{st}$ (labeled by their energy E and lead mode α) which diagonalize the one-body Hamiltonian

$$\sum_j \mathbf{H}_{ij}(0) \Psi_{\alpha E}^{st}(j) = E \Psi_{\alpha E}^{st}(i) \tag{2}$$

and build many-body Slater determinants from these one-body states. For quantities such as the current, this amounts to filling up the energy E with probability $f_\alpha(E)$ (Fermi function of the lead to

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which channel α belongs) which leads to the celebrated Landauer formula for the conductance. Within our notations, the current between sites i and j reads

$$I_{ij} = -\frac{2e}{h}\,\mathrm{Im}\sum_{\alpha}\int dE\, f_\alpha(E)[\Psi^{st}_{\alpha E}(i)]^*\mathbf{H}_{ij}(0)\Psi^{st}_{\alpha E}(j). \tag{3}$$

This approach is by now so standard that $\Psi^{st}_{\alpha E}$ can be obtained directly from open source softwares such as the Kwant package [11]. The generalization of the above approach to time-dependent phenomena is in fact straightforward: one simply follows the evolution of the scattering states upon switching on the time-dependent perturbation and solves

$$i\hbar\frac{\partial}{\partial t}\Psi_{\alpha E}(i,t) = \sum_j \mathbf{H}_{ij}(t)\Psi_{\alpha E}(j,t) \tag{4}$$

with the initial condition:

$$\Psi_{\alpha E}(i,t=0) = \Psi^{st}_{\alpha E}(i). \tag{5}$$

The time-dependent current is now given by

$$I_{ij}(t) = -\frac{2e}{h}\,\mathrm{Im}\sum_{\alpha}\int dE\, f_\alpha(E)[\Psi_{\alpha E}(i,t)]^*\mathbf{H}_{ij}(t)\Psi_{\alpha E}(j,t). \tag{6}$$

Eq. (4) is transparent physically but not directly useful for numerical computations as the wave-function $\Psi_{\alpha E}(i,t)$ is a vector of infinite size. However, by studying the *deviation* between $\Psi_{\alpha E}(i,t)$ and $\Psi^{st}_{\alpha E}(i)e^{-iEt}$ one obtains a finite vector amenable to a numerical solution [8]. In order to prove that Eqs. (4)–(6) lead to the correct generalization of the Landauer formula, Ref. [8] proved its mathematical equivalence with the Wingreen–Meir [12] approach based on the Keldysh formalism. One can also prove that the $\Psi_{\alpha E}(i,t)$ are well defined scattering states, i.e. have the correct structure of superposition of incoming and outgoing states in the leads. The Pauli principle is fully enforced within this scheme, as the initial orthogonality relations of the states are preserved by the unitary evolution of Schrödinger equation. It is interesting to contrast the above set of equations with studies where a (usually Gaussian) wavepacket is propagated through the system. *In fine*, the dynamical equation solved is actually the same. There are however two crucial differences: the initial boundary condition (delocalized over the infinite system in our case) and the final integration over energy which restores the fermionic statistics. The approach presented here is fully many-body and treats Pauli principle exactly.

3. Quantum noise

We now discuss how the approach outlined above can be generalized to calculate the noise properties of a general mesoscopic system subject to time-dependent perturbation. We will focus in particular on the variance of the total number of particles $\hat{n}_\mu$ sent through an electrode μ. This quantity is of special interest to us as it is relatively easy to measure experimentally (upon sending repeated pulses it is essentially a d.c. measurement as opposed to much more challenging high frequency measurements) and it is *conserved and gauge invariant* in Markus' sense [8].

3.1. General expressions

The current operator is defined as a sum of the local currents flowing through a cross section corresponding to an electrode μ (in practice μ is the collection of hopping elements that connect the central system to the electrode)

$$\hat{I}_\mu(t) = \sum_{\langle i,j\rangle\in\mu}\mathbf{H}_{ij}(t)c_i^\dagger(t)c_j(t) - \mathbf{H}_{ji}(t)c_j^\dagger(t)c_i(t), \tag{7}$$

and we define the current–current correlation function as

$$S_{\mu\nu}(t,t') = \langle(\hat{I}_\mu(t) - \langle\hat{I}_\mu(t)\rangle)\times(\hat{I}_\nu(t') - \langle\hat{I}_\nu(t')\rangle)\rangle. \tag{8}$$

The calculation of Eq. (8) requires the statistical average of products of four fermionic operators which is directly obtained using the Wick theorem and the expressions for the one-particle Green's function that were derived in [8]

$$\langle c_j^\dagger(t')c_i(t)\rangle = \sum_\alpha\int\frac{dE}{2\pi}f_\alpha(E)\Psi^*_{\alpha E}(j,t')\Psi_{\alpha E}(i,t) \tag{9}$$

$$\langle c_i(t)c_j^\dagger(t')\rangle = \sum_\alpha\int\frac{dE}{2\pi}(1-f_\alpha(E))\Psi_{\alpha E}(i,t)\Psi^*_{\alpha E}(j,t'). \tag{10}$$

One obtains

$$S_{\mu\nu}(t,t') = \sum_{\alpha,\beta}\int\frac{dE}{2\pi}\int\frac{dE'}{2\pi}f_\alpha(E)(1-f_\beta(E'))I_{\mu,EE'}(t)[I_{\nu,EE'}(t')]^*, \tag{11}$$

with the quantity $I_{\mu,EE'}(t)$ closely related to the initial current operator:

$$I_{\mu,EE'}(t) = \sum_{\langle i,j\rangle\in\mu}[\Psi^*_{\beta E'}(i,t)H_{ij}(t)\Psi_{\alpha E}(j,t) - \Psi^*_{\beta E'}(j,t)H_{ji}(t)\Psi_{\alpha E}(i,t)]. \tag{12}$$

Eqs. (11) relates the typical output of a time-dependent simulation (right-hand side) to the correlation properties (left-hand side). To proceed, we focus on the total number of transmitted particles $\hat{n}_\mu$ over a duration Δ:

$$\hat{n}_\mu = \int_{-\Delta/2}^{\Delta/2}dt\,\hat{I}_\mu(t). \tag{13}$$

With these notations, the average and variance of $\hat{n}_\mu$ are given by

$$\langle\hat{n}_\mu\rangle = \sum_\alpha\int\frac{dE}{2\pi}f_\alpha(E)N_{EE} \tag{14}$$

$$\mathrm{var}(\hat{n}_\mu) = \sum_{\alpha,\beta}\int\frac{dE}{2\pi}\int\frac{dE'}{2\pi}f_\alpha(E)(1-f_\beta(E'))|N_{EE'}|^2, \tag{15}$$

with

$$N_{EE'} = \int_{-\Delta/2}^{\Delta/2}dt\,I_{\mu,EE'}(t). \tag{16}$$

For a finite Δ, the above equations are well defined. However, as we shall see, the noise is totally dominated by the equilibrium noise which diverges at large Δ so that the numerical computation of the excess noise (the quantity which is usually measured) can become problematic. Ultimately, we would like to consider the limit where Δ is infinite. To proceed, we separate the equilibrium physics from the time-dependent one and introduce $\bar{\Psi}_{\alpha E}(i,t)$ which measures how the wave-function deviates from its stationary solution:

$$\Psi_{\alpha E}(i,t) = \Psi^{st}_{\alpha E}(i,t)e^{-iEt} + \bar{\Psi}_{\alpha E}(i,t) \tag{17}$$

$\bar{\Psi}_{\alpha E}(i,t)$ is actually the direct output of the techniques discussed in [8]. With these notations, one can perform the integration over time (in the limit of large Δ) and write the noise in terms of well behaved (converging) integrals. The variance of $\hat{n}_\mu$ now reads

$$\mathrm{var}(\hat{n}_\mu) = \sigma_{st}^2\,\Delta + 2\sigma_{mix} + \bar{\sigma}^2 + O(1/\Delta) \tag{18}$$