Applications of the Nonequilibrium Kubo Formula to the Detection of Quantum Noise

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Abstract. The Kubo fluctuation-dissipation theorem relates the current fluctuations of a system in an equilibrium state with the linear AC-conductance. This theorem holds also out of equilibrium provided that the system is in a stationary state and that the linear conductance is replaced by the (dynamic) conductance with respect to the non equilibrium state. We provide a simple proof for that statement and then apply it in two cases.

We first show that in an excess noise measurement at zero temperature, in which the impedance matching is maintained while driving a mesoscopic sample out of equilibrium, it is the nonsymmetrized noise power spectrum which is measured, even if the bare measurement, i.e. without extracting the excess part of the noise, obtains the symmetrized noise.

As a second application we derive a commutation relation for the two components of fermionic or bosonic currents which holds in every stationary state and which is a generalization of the one valid only for bosonic currents. As is usually the case, such a commutation relation can be used e.g. to derive Heisenberg uncertainty relationships among these current components.

1 Introduction: Definitions, Kubo formula

Consider first a system in an equilibrium state and its current operator defined by:

\[
I = \frac{1}{L} \int_{L^3} dx j(x)
\]

where

\[
j(x) = \frac{e}{2m} \sum \left( P_i \delta(x - x_i) + \delta(x - x_i) P_i \right).
\]

\(e\) is the charge of each of the particles in the system, \(P_i\) its momentum and \(x_i\) its position. We consider the current in a cube of volume \(L^3\). For simplicity we take \(L^3\) to be a unit cube, \(L = 1\), and write our formulae in one dimension.\[1\]

The current fluctuations are often described by the noise power spectrum defined by

\[
S(\omega) = \int_{-\infty}^{\infty} dt e^{i \omega t} \langle I(0) I(t) \rangle.
\]
\langle \ldots \rangle \text{ denotes averaging with respect to a stationary state:}

\[ \langle A \rangle = Tr \rho_0 A \]  

where \( \rho_0 \) is a time independent density matrix:

\[ \dot{\rho}_0 = 0, \quad [H, \rho_0] = 0 \]  

and \( H \) is the Hamiltonian.

Suppose now that the system is driven out of equilibrium by applying an AC electric field

\[ E(t) = E e^{i\omega t}. \]  

For a weak enough \( E(t) \) (this regime is called the linear response regime) the resulting current will be of the form

\[ I(t) = \sigma(\omega) E e^{i\omega t} \]  

where \( \sigma(\omega) \) is time independent. We define the conductance of the system, \( G_d(\omega) \), by

\[ G_d(\omega) = Re \sigma(\omega). \]  

In more general situations, one can perturb the system by various external fields and measure other properties beside the electrical current. In such cases \( G_d(\omega) \), (or \( \sigma(\omega) \)) is called the linear-response coefficient. Here we shall focus on the electrical current but our discussion is extendable to the general case.

Let \( S_{eq}(\omega) \) denote \( S(\omega) \) of a system in equilibrium. In 1956 Kubo \[2-4\] derived a fluctuation-dissipation theorem which relates \( G_d(\omega) \), and \( S_{eq}(\omega) \). It is the following:

\[ S_{eq}(\omega) - S_{eq}(-\omega) = 2\hbar \omega G_d(\omega). \]  

Justifiably, Kubo called it a fluctuation-dissipation relation since it relates the dissipative properties of the system, \( G_d(\omega) \), with its equilibrium fluctuations. There exists also another relation of this type which was derived by Callen and Welton \[5\] in 1951, and which is widely known as the fluctuation-dissipation theorem. It is:

\[ \frac{1}{2}(S_{eq}(\omega) + S_{eq}(-\omega)) = 2G_d(\omega)(\frac{\hbar \omega}{2} + \frac{\hbar \omega}{e\hbar \omega / k_B T - 1}) \]  

where \( T \) is the temperature. On one hand, the Callen-Welton relation is valid only for a system in equilibrium. On the other hand, in his work Kubo stressed that Eq.\[8\] enables a prediction of a nonequilibrium property such as the conductance by a calculation of an equilibrium one \[9\] (Although he did not rule out generalization to nonequilibrium). These are probably the two main reasons why it is often believed that Eq.\[9\] is not valid for nonequilibrium states.
However, Eq.9 is valid in any nonequilibrium state \([7,8,9]\) provided that this state is stationary. That is,

\[
S(-\omega) - S(\omega) = 2\hbar \omega \tilde{G}_d(\omega).
\]  

(11)

Here \(S(\omega)\) is given by Eq.8 at any stationary nonequilibrium state (i.e. with the condition \(5\)). \(\tilde{G}_d(\omega)\) is the response with respect to a small perturbation which is applied to the system which is already driven out of equilibrium by another, not necessarily small, perturbation. Like Eq.9 Eq.11 holds also for interacting systems.

For example, consider a mesoscopic system at zero temperature which is driven out of equilibrium by an external DC field. As a result a DC current arises. \(S(\omega)\) will then be the nonsymmetrized shot-noise spectrum related to this current. Suppose now that an additional small "tickling" AC field \(E(t) = E e^{i\omega t}\) is applied on top of the DC one. As a result also an additional current appears:

\[
\Delta I(t) \equiv \langle I(t) \rangle_{E>0} - \langle I \rangle_{E=0} = \tilde{\sigma}(\omega) E e^{i\omega t}
\]

(12)

and now

\[
\tilde{G}_d(\omega) = \text{Re} \tilde{\sigma}(\omega),
\]

(13)

that is, \(\tilde{G}_d(\omega)\) will then be the linear coefficient relating the new field with the new current (it is therefore perhaps more appropriate to call it the differential AC-conductance to distinguish it from the one valid when the AC field is applied in equilibrium). Eq.11 relates the shot-noise spectra and this differential AC-conductance.

In section 2 we give a simple, self contained, derivation of Eq.11. In section 3 it is shown that noise measurement setup that measures the symmetrized power spectrum at zero temperature yields the nonsymmetrized one when used in an excess noise measurement (provided that the system-setup impedance matching is kept constant while the system is driven out of equilibrium). This is a direct consequence of Eq.11. In section 4 Eq.11 is used to generalize the canonical commutation relations valid for a current in a boson field to the case of a fermionic one, provided the commutator is replaced by its expectation value in a stationary state.

### 2 Derivation of the nonequilibrium Kubo formula

Eq.11 was obtained in ref. 8 by calculating the net absorption from a classical EM field and using the relation between this dissipation and the conductance. A more mathematical proof is given in Ref.7. Here we present a simple and systematic derivation which follows closely the original one given by Kubo. 8, except that, we do not make use of the specific form of the density matrix has
in equilibrium but only assume it to be time independent as in any stationary state. Consider a system described by the Hamiltonian

\[ H_0 = \sum_{i=1}^{n} \frac{P_i^2}{2m} + V \]  

(14)

where \( V = V(x_1, .., x_n) \). To describe the application of a small external alternating electrical field we rewrite it as usual as

\[ H = \sum_{i=1}^{n} \left( \frac{(P_i - eA(x_i, t))^2}{2m} + V(x_1, .., x_n) \right), \]  

(15)

(throughout this section we take \( c = 1 \)). The scalar potential does not appear since we are using the transverse gauge. In this gauge one has

\[ E(x, t) = -\dot{A}(x, t). \]  

(16)

We write \( A(x_i, t) = \int dx A(x, t) \delta(x_i - x) \) (so now \( A(x, t) \) is no longer an operator since \( x_i \) is in the \( \delta \)-function) and keep only first order term in \( A \). \( H \) becomes

\[ H = \sum_{i=1}^{n} \frac{P_i^2}{2m} + V - \int dx A(x, t) j(x) \]  

(17)

where \( j(x) \) is given by Eq.2. We now assume that \( A(x, t) \) is constant within the cube \( L^3 \), and vanishes outside of it. Adding another part of \( A(x, t) \), simply results in adding the linear response to it, so this assumption is not a restrictive one. It is needed only because we are looking for the conductance which is related to \( I(t) \) given by Eq.1. With the above assumption we have

\[ H = H_0 - A(t) I. \]  

(18)

Since we are looking for a relation for a single frequency \( \omega \) we consider the case in which \( A(t) \) is of the form:

\[ A(t) = Ae^{i\omega t} \]  

(19)

and thus, by Eq.10

\[ E(t) = -i\omega Ae^{i\omega t}. \]  

(20)

By Eq.12 we have\(^1\):

\[ \Delta I(t) = -\tilde{\sigma}(\omega)i\omega Ae^{i\omega t}. \]  

(21)

\(^1I \) appearing in Eq.22 is the same as in Eq.10 i.e., it is the average of \( j(x) \), Eq.2. In the presence of the vector potential the proper (gauge-invariant) current is given by \( j_A(x) = j(x) - \frac{e}{m} \rho(x) A(t) \) where \( \rho(x) = \sum_i \delta(x - x_i) \) is the density and thus one should replace \( I \) by \( I_A \equiv I - \frac{e}{m} QA(t) \) where \( Q \) is the total charge. Since the extra (diamagnetic) term \( \frac{e}{m} QA(t) \) is linear in \( A \) it may affect the linear response. However, by Eq.23 \( \frac{e}{m} QA(t) = i \frac{e}{m} \omega QE(t) \). Because of the \( i \) in front of the real coefficient, \( \frac{e}{m} Q \), this term contributes only to the out-of-phase (non-dissipative) part of the current. In other words, defining (in analogy with Eq.12):

\[ \Delta I_A(t) = \tilde{\sigma}_A(\omega)e^{i\omega t}, \]  

one obtains from all the above \( Re \tilde{\sigma}_A(\omega) = Re \tilde{\sigma}(\omega) \). Only the real part of \( \tilde{\sigma}(\omega) \), \( \tilde{G}_d(\omega) \), appears in Eq.10 and therefore our use of \( I \) instead of \( I_A \) is justified.
\[ \Delta I(t) = Tr\delta\rho(t)I \]

(22)

where

\[ \rho(t) - \rho_0 = \delta\rho(t) \sim O(A) \]

is the change in the density matrix due to switching on the perturbation. The equation of motion of the density matrix is

\[ \dot{\rho}(t) = -\frac{i}{\hbar}[H, \rho(t)]. \]

(24)

Recalling that the same equation holds for \( \rho_0 \), that \( \delta\rho(t) \sim O(A) \), and keeping only first order terms in \( A \) we get

\[ \delta\dot{\rho}(t) = -\frac{i}{\hbar}[H_0, \delta\rho(t)] + \frac{i}{\hbar}A(t)[I, \rho_0]. \]

(25)

Eq. 25 is solved by substituting \( \delta\rho(t) = e^{-\frac{i}{\hbar}H_0 t} \alpha(t)e^{\frac{i}{\hbar}H_0 t} \), solving for \( \alpha(t) \), expressing the result in terms of \( \delta\rho(t) \) and then using Eq. 19. One obtains

\[ \delta\rho(t) = i\hbar \int_0^\infty d\tau A(t-\tau)[I(-\tau), \rho_0] \]

(26)

where

\[ I(t) = e^{\frac{i}{\hbar}H_0 t} Ie^{-\frac{i}{\hbar}H_0 t} \]

(27)

is the Heisenberg current operator of the unperturbed system. Inserting this result into Eq. 22 and using \( TrABC = TrCAB \) one gets

\[ \Delta I(t) = \frac{i}{\hbar} \int_0^\infty d\tau A(t-\tau)\langle[I(0), I(-\tau)]\rangle. \]

(28)

Comparing with Eq. 21 and using Eq. 19 yields

\[ \hbar\omega \tilde{\sigma}(\omega) = -\int_0^\infty d\tau e^{-i\omega\tau}\langle[I(0), I(-\tau)]\rangle. \]

(29)

Finally, taking the real part of the last equation while using \( I^\dagger = I \) and the fact that in a stationary state one has \( \langle I(0)I(-\tau) \rangle = \langle I(\tau)I(0) \rangle \), we obtain

\[ S(-\omega) - S(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau}\langle[I(\tau), I(0)]\rangle = 2\hbar\omega\tilde{G}_d(\omega) \]

(30)

as in Eq. 11.
3 First application. Excess noise measurement

Consider a mesoscopic system at zero temperature coupled to a detection setup (also at zero temperature) which is designed in such a way that it will measure (as is very often assumed) the symmetrized noise spectrum:

\[ S_m(\omega) = S_{sym}(\omega) = \frac{1}{2}(S(\omega) + S(-\omega)). \] (31)

\( S_m(\omega) \) stands for the measured spectrum. Such a setup may resemble, for example, the one used in [10]. In [11] it was shown that for a very broad class of setups, if one subtracts the noise measured at equilibrium from the nonequilibrium one the resulting spectrum will be given by Eq.3 i.e. it will be nonsymmetrized\(^2\). The main assumption used was that the conductance remains approximately unchanged while the system is driven out of equilibrium so that the latter remains impedance-matched to the detector. This ensures that all the extra power emitted by the shot-noise is detected. Claiming that such a measurement yields \( S(\omega) \) may seem to contradict the assumption Eq.31 however we shall now show that there is no inconsistency: Also in the case of Eq.31 the excess measurement yields \( S(\omega) \) and not \( S_{sym}(\omega) \).

By its definition the measured excess noise is

\[ S_{m,\text{excess}}(\omega) \equiv S_m(\omega) - S_{m,eq}(\omega) \] (32)

where \( S_{m,eq}(\omega) \) is the noise measured in equilibrium. Assuming Eq.31 we have

\[ S_{m,\text{excess}}(\omega) = \frac{1}{2}(S(\omega) + S(-\omega)) - \frac{1}{2}(S_{eq}(\omega) + S_{eq}(-\omega)). \] (33)

This can be written as

\[ S_{m,\text{excess}}(\omega) = S(\omega) - S_{eq}(\omega) + \frac{1}{2}(S(-\omega) - S(\omega)) - \frac{1}{2}(S_{eq}(-\omega) - S_{eq}(\omega)). \] (34)

Applying Eq.11 we get

\[ S_{m,\text{excess}}(\omega) = S(\omega) - S_{eq}(\omega) + \hbar \omega (\tilde{G}_d(\omega) - G_d(\omega)). \] (35)

Since we assumed that the conductance remains the same in and out of equilibrium, the last term on the right vanishes. and one is left with

\[ S_{m,\text{excess}}(\omega) = S(\omega) - S_{eq}(\omega). \] (36)

Finally, since \( S(\omega) \) is the emission spectrum [13] and since in equilibrium at zero temperature there is no emission, one has

\[ S_{eq}(\omega) = 0 \quad k_B T = 0 \] (37)

\(^2\)This was shown also for setups that include an amplification stage (as in [10]), which is usually the one determining the measured quantity (see e.g., [15]). For an analysis of a detection without amplification see Refs. [14] and [15].
and thus
\[ S_{m,\text{excess}}(\omega) = S(\omega) \quad k_B T = 0 \] (38)
as asserted in [11]. Thus, also in the specific case of Eq. 31 the excess noise measurement yields the general results Eqs. 36 and 38. We emphasize that contrary to a common view in the literature [14], Eq. 31 is merely a specific case and not a general rule. For a concrete example where Eq. 31 does not hold see Ref. [15].

4 Second application. Commutation relations for fermionic current components

We now apply Eq. 11 in order to obtain commutation relations for fermionic current components. Let us define
\[ I(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt e^{i\omega t} I(t). \] (39)

\[ I(t) \] is hermitian and therefore
\[ I(t) = I(-\omega). \] (40)

In any stationary state one has:

\[ \langle I(\omega) \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle I(t) \rangle \]
\[ = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_i P_i e^{iE_i t} \langle i | I | i \rangle e^{-iE_i t} = \delta(\omega) \sqrt{2\pi} \langle I \rangle, \] (41)

where \( P_i \) is the probability to be in the eigenstate \(|i\rangle\), and

\[ \langle I(\omega)I(\omega') \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dt dt' e^{i\omega t + i\omega' t'} \sum_i P_i e^{iE_i t} \langle i | e^{-iH(t-t')} | i \rangle e^{-iE_i t'}. \] (42)

Defining
\[ \tau_+ = \frac{1}{2}(t + t'), \quad \tau_- = t' - t \]
\[ t = \tau_+ + \frac{1}{2} \tau_-, \quad t' = \tau_+ - \frac{1}{2} \tau_. \]
one has

\[
\langle I(\omega)I(\omega') \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau_- d\tau_+ \sum_i P_i \langle i | e^{iH\tau_-} I(i) e^{-iE_i \tau_-} e^{i(\omega + \omega') \tau_+} e^{i(\omega - \omega') \frac{\tau_+}{2}} | i \rangle
\]

\[
= \int_{-\infty}^{\infty} d\tau_- \langle I e^{iH\tau_-} I e^{-iH\tau_-} \rangle \delta(\omega + \omega') e^{-\frac{1}{2}(\omega - \omega') \tau_-}
\]

\[
= \delta(\omega + \omega') \int_{-\infty}^{\infty} d\tau_- e^{-i\omega \tau_-} \langle I(0)I(\tau_-) \rangle.
\]

(43)

Thus,

\[
\langle I(\omega)I(\omega') \rangle = \delta(\omega + \omega') S(-\omega).
\]

(44)

The averaged cosine and sine components of a current, \( \bar{I}_{cs}(\Omega) \) and \( \bar{I}_{sn}(\Omega) \), are Hermitian operators defined by

\[
\bar{I}_{cs}(\Omega) \equiv \bar{I}(\Omega) + \bar{I}^\dagger(\Omega), \quad \bar{I}_{sn}(\Omega) \equiv -i(\bar{I}(\Omega) - \bar{I}^\dagger(\Omega)),
\]

(45)

where we defined averaging over a frequency bandwidth by

\[
\bar{X}(\Omega) = \int_B d\omega X(\omega) \quad B : [\Omega - \frac{1}{2}\Delta, \Omega + \frac{1}{2}\Delta].
\]

(46)

In a current carried by a boson field, \( \bar{I}_{cs}(\Omega) \) and \( \bar{I}_{sn}(\Omega) \) form a canonical pair similar to \( x \) and \( p \) of an harmonic oscillator (and in that case \( I(\Omega) \) is analogous to the annihilation operator of an harmonic oscillator). That is,

\[
[\bar{I}_{cs}(\Omega), \bar{I}_{sn}(\Omega)] = if(\Omega)
\]

(47)

where \( f(\Omega) \) is a real c-number which may depend on \( \Omega \). An example for such a case is the current field in an ideal transmission line [10, 17]. Eq. (17) allows one to derive uncertainty relations involving the current components which have important consequences in the theory of quantum amplification [18, 19, 20]. However, this equation is generally not valid for a current carried by fermions, in which case the above commutator is in general an operator.

To overcome this problem we shall use Eq. (11). Inserting Eq. (39) into 3, integrating, averaging over the band width \( B \), and making use of Eqs. (40) and (44) one gets

\[
\bar{S}(\Omega) = \langle \bar{I}^\dagger(\Omega)\bar{I}(\Omega) \rangle
\]

\[
\bar{S}(-\Omega) = \langle \bar{I}(\Omega)\bar{I}^\dagger(\Omega) \rangle.
\]

(48)

Subtracting these two equations and making use of Eq. (11) result in

\[
\langle [\bar{I}(\Omega), \bar{I}^\dagger(\Omega)] \rangle = 2\hbar \Omega \bar{G}_d(\Omega) \Delta,
\]

(49)
where for simplicity we assume that $\Delta$ is small enough so that $\tilde{G}_d(\Omega)$ remains constant in it. From Eq. 45 one sees

$$\langle \bar{I}_{cs}(\Omega) \bar{I}_{sn}(\Omega) \rangle = 2i \langle \bar{I}(\Omega), \bar{I}^\dagger(\Omega) \rangle. \quad (50)$$

Combining the last two equations we finally get

$$\langle [\bar{I}_{cs}(\Omega), \bar{I}_{sn}(\Omega)] \rangle = 4i \hbar \Omega \tilde{G}_d(\Omega) \Delta. \quad (51)$$

Thus, we have transformed Eq. 11 into the form of commutation relations which is valid for any current in a stationary state, whether it is carried by fermions or bosons. The usefulness of Eq. 51 stems from the fact that in many cases, the conductance $\tilde{G}_d(\Omega)$ is the same in a large set of stationary states (as e.g. was the case in Sec. 3) and therefore, within such a set, $\bar{I}_{cs}(\Omega)$ and $\bar{I}_{sn}(\Omega)$ possess properties of an ordinary pair of canonical variables.

5 Summary and conclusions

Kubo’s fluctuation dissipation theorem holds also outside of equilibrium, as long as the system is in a stationary state. As a consequence, excess noise measurement of, for example, the symmetrized noise spectrum yields the non-symmetrized one. Another consequence is that although the commutator of the two components of fermionic currents is not in general a purely imaginary constant c-number (unlike for their bosonic counterparts), the projection of their commutator onto all stationary states having the same conductance, is such a c-number. This can be shown to result in Heisenberg constraints on the performance of quantum transistors [21].

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