



PAPER

Current conserving theory for frequency dependent noise power under dc bias

OPEN ACCESS

RECEIVED
13 July 2017REVISED
28 November 2017ACCEPTED FOR PUBLICATION
13 December 2017PUBLISHED
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Keywords: displacement current, scattering matrix theory, shot noise

Abstract

We formulate a current conserving theory for frequency dependent noise power under dc bias. In calculating the noise power we explicitly take into account of the displacement current operator. It is shown that the equilibrium frequency dependent noise satisfies the relation $S_{\text{eq},\alpha\beta}(\omega) = \epsilon(\omega)[G_{\alpha\beta}(\omega) + G_{\beta\alpha}^*(\omega)]$ where $G_{\alpha\beta}(\omega)$ is the frequency dependent conductance including both conduction current and displacement current contribution.

1. Introduction

The equilibrium fluctuation–dissipation theorem which relates the linear conductance to equilibrium noise power is fundamentally important in quantum transport [1–3]. Extensive efforts have been made to extend this theorem to the nonlinear and non-equilibrium regime [4–6]. Fluctuation theorem has been established to relate higher order response function to fluctuations of the systems. The fluctuation–dissipation theorem in ac regime has also been discussed. For instance it has been used to calculate dynamic conductance due to the conduction current [7].

It has been realized that in ac regime the current conserving and gauge invariant conditions are two fundamental requirements for quantum charge transport. It is known that the conduction current alone does not conserve the current under ac bias due to the charge accumulation in the scattering region which is related to the displacement current [8]. In another word, denoting $G_{\alpha\beta}^c(\omega)$ the dynamic conductance due to conduction current, we have $\sum_{\alpha} G_{\alpha\beta}^c(\omega) \neq 0$ and $\sum_{\beta} G_{\alpha\beta}^c(\omega) \neq 0$. By adding a self-consistent Coulomb interaction in the Hamiltonian it will include the contribution of the displacement current and solve the problem of current conservation. Using this approach, the problem of current conservation of dynamic conductance has been solved at low frequencies [8] and finite frequencies [9]. Under dc bias, there is no charge accumulation and the current is conserved since the displacement current is not present.

It is known that in addition to the current, the noise power and higher order moments are needed to characterize the quantum transport process. In another word, the current operator \hat{I}_{α} can be used to generate the current $\langle \hat{I}_{\alpha} \rangle$, noise power³ $S_{\alpha\beta}$, etc. If the current operator is conserved ($\sum_{\alpha} \hat{I}_{\alpha} = 0$), the current, noise power, and higher order moments will be conserved automatically, i.e., $\sum_{\alpha} \langle \hat{I}_{\alpha} \rangle = 0$, $\sum_{\alpha} S_{\alpha\beta} = \sum_{\beta} S_{\alpha\beta} = 0$. Although construction of a current conserving current operator is an unsolved problem, physical insight can be obtained by looking into the issue of the conservation of noise power in ac regime.

For example, the equilibrium frequency dependent noise power is related to the frequency dependent conductance due to the conduction current [10],

$$S_{\text{eq},\alpha\beta}(\omega) = \epsilon(\omega)[G_{\alpha\beta}^c(\omega) + G_{\beta\alpha}^{c*}(\omega)], \quad (1)$$

where $\epsilon(\omega) = \omega \frac{e^{\omega/kT} + 1}{e^{\omega/kT} - 1}$ is defined in [10]. At zero frequency, the equilibrium fluctuation–dissipation theorem gives $S_{\text{eq},\alpha\beta} = 2kT[G_{\alpha\beta} + G_{\beta\alpha}^*]$ where $G_{\alpha\beta} = G_{\alpha\beta}^c(0)$ and $S_{\alpha\beta}^{\text{eq}} = S_{\text{eq},\alpha\beta}(0)$ are dc conductance and dc noise

³ The symmetric noise power can be defined as $S_{\alpha\beta}(t, t') = (1/2)[\langle \Delta \hat{I}_{\alpha}(t) \Delta \hat{I}_{\beta}(t') + \Delta \hat{I}_{\beta}(t') \Delta \hat{I}_{\alpha}(t) \rangle]$ where $\Delta \hat{I}_{\alpha} = \hat{I}_{\alpha} - \langle \hat{I}_{\alpha} \rangle$.

power respectively. For current in the linear response regime, we have $I_\alpha = \sum_\beta G_{\alpha\beta} v_\beta$ where α and β denote the lead and v_β is the bias voltage of lead β . Current conservation corresponds to $\sum_\alpha I_\alpha = 0$ which leads to the current conserving condition $\sum_\alpha G_{\alpha\beta} = 0$. Since the bias is defined up to an additive constant which does not affect the current, i.e., $I_\alpha = \sum_\beta G_{\alpha\beta} (v_\beta + v_0)$, this gives rise to the gauge invariant condition $\sum_\beta G_{\alpha\beta} = 0$. This in turn gives conservation condition for the noise power, $\sum_\alpha S_{\alpha\beta}^{\text{eq}} = \sum_\beta S_{\alpha\beta}^{\text{eq}} = 0$. Since the dynamic conductance $G_{\alpha\beta}^c(\omega)$ due to the conduction current is not conserved, from equation (1) the noise power is not conserved at finite frequencies.

Clearly there is an inconsistency in the frequency dependent fluctuation–dissipation relation equation (1). On one hand, we have a current conserving theory for dynamic conductance [8, 9]. On the other hand our existing theory of frequency dependent equilibrium noise power equation (1) is not conserved. It is the purpose of this paper to address the issue of noise power conservation.

It turns out that adding the self-consistent Coulomb interaction in the Hamiltonian will not conserve the noise power. If we want to discuss the fluctuation of the current (noise power), we have to treat the current as an operator which is a stochastic quantity that can fluctuate and has its distribution. From this point of view, the current operator under dc bias is not conserved in general and the displacement current operator must play a role. While it is clear that the average value of the displacement current operator is zero under dc bias, the fluctuation of the displacement current can not be neglected even under dc bias if the noise power is considered. As we will show below, the missing of the displacement current operator is responsible for the violation of the finite frequency noise power conservation.

In this paper, we develop a phenomenological theory for the displacement current operator and show that the equilibrium noise power is conserved by including the displacement current operator.

2. Theoretical formalism

2.1. Scattering matrix theory

To pave the way for the discussion, we first briefly review the scattering matrix theory (SMT) developed by Büttiker to calculate the frequency dependent noise power under dc bias. The current operator in frequency domain in SMT is given by ($e = 1$ and $\hbar = 1$) [11]

$$\hat{I}_\alpha^c(\omega) = \int \frac{dE}{2\pi} \sum_{\beta\gamma} \hat{a}_\beta^\dagger(E) \hat{a}_\gamma(\bar{E}) A_{\beta\gamma}(\alpha, E, \bar{E}), \quad (2)$$

where a_β^\dagger is the creation operator for the electron incident from lead β , $\bar{E} = E + \omega$ and the matrix A is defined as [11]

$$A_{\beta\gamma}(\alpha, E, \bar{E}) = \delta_{\alpha\beta} \delta_{\alpha\gamma} - s_{\alpha\beta}^\dagger(E) s_{\alpha\gamma}(\bar{E}), \quad (3)$$

where $s_{\alpha\beta}(E)$ is the scattering matrix from lead β to lead α . To distinguish the current in equation (2) from the displacement current introduced later, we have denoted this current as the conduction current with superscript c . Using the relation $\langle \hat{a}_\alpha^\dagger(E) \hat{a}_\beta(E') \rangle = \delta_{\alpha\beta} \delta(E - E') f_\alpha(E)$, where $\langle \dots \rangle$ denotes the quantum average and $f_\alpha(E)$ is the Fermi distribution function of the lead α , the average current is found to be

$$\langle \hat{I}_\alpha^c(\omega) \rangle = \delta(\omega) \int \frac{dE}{2\pi} \sum_{\beta} f_\beta(E) A_{\beta\beta}(\alpha, E, E). \quad (4)$$

After the Fourier transform with respect to frequency, we find the time independent current,

$$I_\alpha^c = \langle \hat{I}_\alpha^c \rangle = \int \frac{dE}{2\pi} \sum_{\beta} f_\beta(E) A_{\beta\beta}(\alpha, E, E), \quad (5)$$

which is the well known Landauer–Büttiker formula. Using the relation

$$\sum_{\alpha} A_{\beta\gamma}(\alpha, E, E) = 0, \quad (6)$$

valid for any β and γ , we verify that the current under dc bias is conserved, i.e., $\sum_{\alpha} I_\alpha^c = 0$.

The fluctuations of the current away from their average value are characterized by the noise power $S_{\alpha\beta}$. Under dc bias $S_{\alpha\beta}$ is found to be [12]

$$S_{\alpha\beta}(\omega) = \int \frac{dE}{2\pi} \sum_{\gamma\delta} A_{\gamma\delta}(\alpha, E, \bar{E}) \times A_{\delta\gamma}(\beta, \bar{E}, E) F_{\gamma\delta}(E, \bar{E}), \quad (7)$$

where

$$F_{\gamma\delta}(E, \bar{E}) = f_\gamma(E)(1 - f_\delta(\bar{E})) + f_\delta(\bar{E})(1 - f_\gamma(E)). \quad (8)$$

We now examine current conservation of equation (7). Since $\bar{E} = E$ at $\omega = 0$, equation (6) gives

$$\sum_{\alpha} S_{\alpha\beta}(0) = \sum_{\beta} S_{\alpha\beta}(0) = 0, \quad (9)$$

showing that the zero-frequency noise is conserved. At finite frequencies, however, noise power under dc bias is not conserved anymore which has been recognized long time ago by Büttiker [10].

The issue of the conservation of noise power is rooted from the current conservation condition of current operator. From equation (6) we immediately have

$$\sum_{\alpha} \hat{I}_{\alpha}^c(\omega = 0) = 0, \quad (10)$$

which leads to equation (9). When ω is nonzero, $\sum_{\alpha} \hat{I}_{\alpha}^c(\omega) = 0$ is not valid and therefore the conservation condition is violated for the finite frequency noise power. As we mentioned previously, the missing component is the displacement current operator which will be discussed below.

2.2. Displacement current operator

Now we present a phenomenological theory for displacement current operator. To demonstrate this method, we will treat equilibrium noise power in this paper. The non-equilibrium noise power can be dealt with similarly. We start with the self-consistent formalism for current operator,

$$\hat{I}_{\alpha}(\omega) = \hat{I}_{\alpha}^c(\omega) + \hat{I}_{\alpha}^d(\omega), \quad (11)$$

where $\hat{I}_{\alpha}^c(\omega)$ is the current operator for the conduction current defined in equation (2). The displacement current operator $\hat{I}_{\alpha}^d(\omega)$ is the induced current due to Coulomb interaction. On the Hartree level and in the linear response regime it is assumed to be⁴.

$$\hat{I}_{\alpha}^d(\omega) = i\omega \int dx \frac{d\bar{n}_{\alpha}(\omega, x)}{dE} \hat{U}(\omega, x), \quad (12)$$

where $d\bar{n}_{\alpha}(\omega, x)/dE$ is the frequency-dependent emissivity describing the local density of states (DOS) for electrons exiting to lead α [9], and $\hat{U}(\omega, x)$ is the Coulomb potential operator due to quantum fluctuation given by [10]

$$\hat{U}(\omega, x) = \int dx' g(\omega, x, x') \hat{N}(\omega, x'), \quad (13)$$

where $g(\omega, x, x')$ is the Coulomb potential response function or Green's function and $\hat{N}(\omega, x)$ is the number operator in the scattering region. The Coulomb potential response function $g(\omega, x, x')$ satisfies the Poisson-like equation,

$$-\nabla_x^2 g(\omega, x, x') = 4\pi\delta(x - x') - 4\pi \int dx'' \Pi(\omega, x, x'') g(\omega, x'', x'), \quad (14)$$

where $\Pi(\omega, x, x')$ is the Lindhard function [8, 9]. The physical meaning of this equation is clear. The first term on the right-hand side of this equation is the point charge source term and the second term is the induced charge due to the Coulomb interaction. To find the equation governing the Coulomb potential operator $\hat{U}(\omega, x)$, we express it in terms of $\hat{a}_{\alpha}^{\dagger}$ and \hat{a}_{α} [10]

$$\hat{U}(\omega, x) = \sum_{\beta\gamma} \int \frac{dE}{2\pi} \hat{a}_{\beta}^{\dagger}(E) \hat{a}_{\gamma}(\bar{E}) u_{\beta\gamma}(E, \omega, x), \quad (15)$$

where the Coulomb potential matrix $u_{\beta\gamma}$ will be discussed later. We now derive an expansion for $\hat{N}(\omega, x)$ similar to equation (15) and the poisson like equation for $u_{\beta\gamma}$.

The number operator $\hat{N}(t, x)$ in time domain is defined as follows

$$\hat{N}(t, x) = \sum_{\beta\gamma} \frac{1}{2\pi\sqrt{v_{\beta}v_{\gamma}}} \hat{\Psi}_{\beta}^{\dagger}(t, x) \hat{\Psi}_{\gamma}(t, x), \quad (16)$$

the normalization in this equation is defined so as to obtain the familiar result of average number of particle (see equation (21)). Here

$$\hat{\Psi}_{\beta}(t, x) = \int dE e^{-iEt} \psi_{\beta}^{(\text{out})}(E, x) \hat{a}_{\beta}(E), \quad (17)$$

where $\psi_{\beta}^{(\text{out})}(E, x)$ is the outgoing wave function for electrons coming from lead β . After the Fourier transformation, we have

⁴ Similar displacement current operator has been proposed for mesoscopic capacitors in [10].

$$\hat{N}(\omega, \mathbf{x}) = \int \frac{dE}{2\pi} \sum_{\beta\gamma} \hat{a}_{\beta}^{\dagger}(E) \hat{a}_{\gamma}(\bar{E}) n_{\beta\gamma}(E, \omega, \mathbf{x}), \quad (18)$$

where [10]

$$n_{\beta\gamma}(E, \omega, \mathbf{x}) = \frac{1}{\sqrt{v_{\beta}v_{\gamma}}} \psi_{\beta}^{*(\text{out})}(E, \mathbf{x}) \psi_{\gamma}^{(\text{out})}(\bar{E}, \mathbf{x}), \quad (19)$$

is the frequency dependent partial local DOS associated with electrons entering from lead β and γ and v_{β} is the electron velocity in lead β . It can be shown in the [appendix](#) that the following relation holds (see derivation below equation (48))

$$\int d\mathbf{x} n_{\beta\gamma}(E, \omega, \mathbf{x}) = \frac{i}{\omega} \sum_{\alpha} A_{\beta\gamma}(\alpha, E, \bar{E}) = N_{\beta\gamma}(E, \omega), \quad (20)$$

where $N_{\beta\gamma}(E, \omega)$ is the partial DOS defined in [13]. It describes the DOS for electrons coming from lead β and γ . Note that taking quantum average on $\hat{N}(\omega, \mathbf{x})$ we obtain the familiar result

$$\langle \hat{N}(\omega, \mathbf{x}) \rangle = \sum_{\beta} \frac{1}{v_{\beta}} \int dE |\psi_{\beta}^{(\text{out})}(E, \mathbf{x})|^2 f_{\beta}(E) \delta(\omega). \quad (21)$$

From equations (2), (18) and (20) we have the continuity equation for current and number operators⁵

$$\sum_{\alpha} \hat{I}_{\alpha}^c(\omega) + i\omega \int d\mathbf{x} [\hat{N}(\omega, \mathbf{x})] = 0. \quad (22)$$

We can define another frequency dependent partial local DOS (emissivity) that can be expressed as follows,

$$\bar{n}_{\beta\gamma}(E, \omega, \mathbf{x}) = \frac{1}{\sqrt{v_{\beta}v_{\gamma}}} \psi_{\gamma}^{*(\text{in})}(\bar{E}, \mathbf{x}) \psi_{\beta}^{(\text{in})}(E, \mathbf{x}), \quad (23)$$

where $\psi_{\gamma}^{(\text{in})}(E, \mathbf{x})$ is the incoming wave function for electrons coming from lead γ (its definition is given in [appendix](#)). A similar relation holds for emissivity,

$$\int d\mathbf{x} [\bar{n}_{\beta\gamma}(E, \omega, \mathbf{x})] = \frac{i}{\omega} \sum_{\alpha} A_{\beta\gamma}(\alpha, E, \bar{E}), \quad (24)$$

Now the local injectivity $dn_{\alpha}(\omega, \mathbf{x})/dE$ and the local emissivity $d\bar{n}_{\alpha}(\omega, \mathbf{x})/dE$ defined in [9] can be expressed as

$$\frac{dn_{\alpha}(\omega, \mathbf{x})}{dE} = \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} n_{\alpha\alpha}(E, \omega, \mathbf{x}), \quad (25)$$

and

$$\frac{d\bar{n}_{\alpha}(\omega, \mathbf{x})}{dE} = \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \bar{n}_{\alpha\alpha}(E, \omega, \mathbf{x}), \quad (26)$$

from which we have local DOS $dn(\omega, \mathbf{x})/dE = \sum_{\alpha} dn_{\alpha}(\omega, \mathbf{x})/dE$ and $d\bar{n}(\omega, \mathbf{x})/dE = \sum_{\alpha} d\bar{n}_{\alpha}(\omega, \mathbf{x})/dE$.

Using equations (13), (15) and (18) we immediately have

$$\mathbf{u}_{\beta\gamma}(E, \omega, \mathbf{x}) = \int d\mathbf{x}' g(\omega, \mathbf{x}, \mathbf{x}') n_{\beta\gamma}(E, \omega, \mathbf{x}'), \quad (27)$$

from which we find the poisson-like equation governing the Coulomb interaction matrix $\mathbf{u}_{\beta\gamma}$,

$$\begin{aligned} & -\nabla_x^2 \mathbf{u}_{\beta\gamma}(E, \omega, \mathbf{x}) + 4\pi \int d\mathbf{x}' \Pi(\omega, \mathbf{x}, \mathbf{x}') \mathbf{u}_{\beta\gamma}(E, \omega, \mathbf{x}') \\ & = 4\pi n_{\beta\gamma}(E, \omega, \mathbf{x}). \end{aligned} \quad (28)$$

The characteristic potential u_{α} used in [9, 11] can be defined as $u_{\alpha} = \int (dE/2\pi) u_{\alpha\alpha}(f - \bar{f})/\omega$. From equation (25), we find the familiar poisson-like equation for the characteristic potential u_{α} ,

⁵ The continuity equation can also be obtained from the equation of motion showing the consistency of our theory (see equation (65) of [18]).

$$\begin{aligned}
& -\nabla_x^2 u_\alpha(\omega, x) + 4\pi \int dx' \Pi(\omega, x, x') u_\alpha(\omega, x') \\
& = 4\pi \frac{dn_\alpha(\omega, x)}{dE}.
\end{aligned} \tag{29}$$

To the linear order the Coulomb potential is related to the characteristic potential as $U = \sum_\alpha u_\alpha v_\alpha$ where v_α is the bias voltage at lead α . The gauge invariant condition gives [8] $\sum_\alpha u_\alpha = 1$.

To avoid possible confusion, we emphasize that quantities such as $n_{\beta\gamma}$ and $u_{\beta\gamma}$ with double subscript depend on energy E and do not depend on temperature while the quantities dn_α/dE and u_α depend on temperature and Fermi energy E_F .

2.3. Reciprocity relation

Note that the injectivity and emissivity defined above are the same as those defined in the linear response theory and obey the reciprocity relation [9], from which we have $d\bar{n}_\alpha(\omega, x, B)/dE = dn_\alpha(\omega, x, -B)/dE$, $\Pi(\omega, B, x, x') = \Pi(\omega, -B, x', x)$ and $g(\omega, B, x, x') = g(\omega, -B, x', x)$. The gauge invariant condition in the linear response theory requires $\sum_\alpha u_\alpha(\omega, x, \pm B) = 1$ from which we obtain

$$\int dx' g(\omega, x, x') \frac{dn(\omega, x')}{dE} = 1, \tag{30}$$

and

$$\int dx' \frac{d\bar{n}(\omega, x')}{dE} g(\omega, x', x) = 1. \tag{31}$$

In the absence of magnetic field, equations (19) and (23) are the same quantity, which shows that injectivity and emissivity are the same in the absence of magnetic field.

2.4. Current conservation at operator level

We now examine the current conservation condition at operator level. Substituting equation (13) into (12) and using equation (31) we arrive at

$$\sum_\alpha \hat{I}_\alpha^d(\omega) = i\omega \int dx [\hat{N}(\omega, x)], \tag{32}$$

which says that the sum of displacement current equals to the rate of change of total charges in the scattering region. From the continuity equations (22) and (32) we see that the total current operator conserves the current, i.e., $\sum_\alpha (\hat{I}_\alpha^c(\omega) + \hat{I}_\alpha^d(\omega)) = 0$.

With the displacement current operator defined, the total current operator in equation (11) can be written as

$$\hat{I}_\alpha(\omega) = \int \frac{dE}{2\pi} \sum_{\beta\gamma} \hat{a}_\beta^\dagger(E) \hat{a}_\gamma(\bar{E}) A_{\beta\gamma}^t(\alpha, E, \bar{E}), \tag{33}$$

where

$$A_{\beta\gamma}^t(\alpha, E, \bar{E}) = A_{\beta\gamma}(\alpha, E, \bar{E}) + i\omega \int dx \frac{d\bar{n}_\alpha(\omega, x)}{dE} u_{\beta\gamma}(E, \omega, x), \tag{34}$$

where $u_{\beta\gamma}(E, \omega, x) = \int dx' g(\omega, x, x') n_{\beta\gamma}(E, \omega, x')$ (see equation (27)).

Now it is easy to confirm explicitly the conservation of current at the operator level by showing $\sum_\alpha A_{\beta\gamma}^t(\alpha, E, \bar{E}) = 0$ which is obvious from equations (20) (27), and (31). So by introducing a fluctuating Coulomb potential, the frequency dependent current operator is conserved to all orders of dc bias. This ensures that noise power as well as higher order moments satisfy the conservation condition to all orders of dc bias. Changing ω to $-\omega$ in equation (33) and shifting E to $E + \omega$, we have

$$A_{\beta\gamma}^t(\alpha, \bar{E}, E) = A_{\beta\gamma}(\alpha, \bar{E}, E) - i\omega \int dx \left(\frac{d\bar{n}_\alpha(\omega, x)}{dE} \right)^* u_{\beta\gamma}^*(E, \omega, x). \tag{35}$$

We can also show that $\sum_\alpha A_{\beta\gamma}^t(\alpha, \bar{E}, E) = 0$.

2.5. Noise power

Now we evaluate the equilibrium state noise spectrum. From [11], we have

$$\begin{aligned}
S_{\alpha\beta}(\omega) &= \int \frac{dE}{2\pi} \sum_{\gamma\delta} A_{\gamma\delta}^t(\alpha, E, \bar{E}) \\
&\quad \times A_{\delta\gamma}^t(\beta, \bar{E}, E) E_{\gamma\delta}(E, \bar{E}),
\end{aligned} \tag{36}$$

where

$$E_{\gamma\delta}(E, \bar{E}) = f_{\gamma}(E)(1 - f_{\delta}(\bar{E})) + f_{\delta}(\bar{E})(1 - f_{\gamma}(E)). \quad (37)$$

In the equilibrium state the Fermi distribution functions of the different leads are the same, i.e., $f_{\gamma}(E) = f_{\delta}(E) = f(E)$. From equations (34) and (35) the equilibrium noise is given by

$$S_{\text{eq},\alpha\beta}(\omega) = \epsilon(\omega)[S_{\text{eq},\alpha\beta}^{(1)}(\omega) + S_{\text{eq},\alpha\beta}^{(2)}(\omega)]. \quad (38)$$

In equation (38) the first term can be expressed in terms of the dynamical frequency dependent conductance $G_{\alpha\beta}(\omega)$

$$S_{\text{eq},\alpha\beta}^{(1)}(\omega) = G_{\alpha\beta}(\omega) + G_{\beta\alpha}^*(\omega), \quad (39)$$

with

$$G_{\alpha\beta}(\omega) = \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} [\delta_{\alpha\beta} - s_{\alpha\beta}^{\dagger}(E)s_{\alpha\beta}(\bar{E})] + i\omega \text{Tr} \left[\frac{d\bar{n}_{\alpha}(\omega)}{dE} u_{\beta}(\omega) \right], \quad (40)$$

where $f = f(E)$ and $\bar{f} = f(\bar{E})$. The second term $S_{\text{eq},\alpha\beta}^{(2)}(\omega)$ is given by

$$S_{\text{eq},\alpha\beta}^{(2)}(\omega) = i\omega \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} (s_{\alpha\gamma}^{\dagger}(E)s_{\alpha\delta}(\bar{E})) \times \text{Tr} \left[\left(\frac{d\bar{n}_{\beta}(\omega)}{dE} \right)^* u_{\delta\gamma}^*(\omega) \right] - s_{\beta\delta}^{\dagger}(\bar{E})s_{\beta\gamma}(E) \text{Tr} \left[\frac{d\bar{n}_{\alpha}(\omega)}{dE} u_{\gamma\delta}(\omega) \right] - i\omega \text{Tr} \left[\left(\frac{d\bar{n}_{\beta}(\omega)}{dE} \right)^* u_{\gamma\delta}^*(\omega) \right] \text{Tr} \left[\frac{d\bar{n}_{\alpha}(\omega)}{dE} u_{\gamma\delta}(\omega) \right]. \quad (41)$$

We will show in the [appendix](#) that $S_{\text{eq},\alpha\beta}^{(2)}(\omega) = 0$. Hence the frequency dependent equilibrium noise is proportional to the dynamical frequency dependent conductance,

$$S_{\text{eq},\alpha\beta}(\omega) = \epsilon(\omega)[G_{\alpha\beta}(\omega) + G_{\beta\alpha}^*(\omega)], \quad (42)$$

which is the frequency dependent equilibrium fluctuation–dissipation theorem. As shown in [9] the dynamic conductance $G_{\alpha\beta}(\omega)$ is current conserving and gauge invariant, i.e., $\sum_{\alpha} G_{\alpha\beta}(\omega) = \sum_{\beta} G_{\alpha\beta}(\omega) = 0$ leading to a conserved noise power in equation (42).

So far, we have discussed the noise power using the symmetric definition (see footnote 3). Experimentally, the measurable quantity is usually non-symmetric [14, 15] It was derived in [14] that the experimental response of current–current correlator is given by

$$S = K[S_+ + N_{\omega}(S_+ - S_-)] \quad (43)$$

with $S_+(\omega) = \int dt \langle \hat{I}(0)\hat{I}(t) \rangle \exp(i\omega t)$ and $S_- = \int dt \langle \hat{I}(t)\hat{I}(0) \rangle \exp(i\omega t)$, K is a constant, and $N_{\omega} = 1/[\exp(\hbar\omega/kT) - 1]$. It is straightforward to show that our theory also applies to non-symmetric noise power. We only need to modify the function $\epsilon(\omega)$ in equation (1) or equation (39).

In this work, we used the SMT developed by Buttiker [11] in 1992. Equation (2) is valid provided that the frequency is much smaller than the Fermi energy. However, when frequency is very large, one could use a more realistic expression for current operator which is spacial dependent [16].

In this paper, we have included the displacement current operator only in the linear order in bias voltage which already makes the current operator conserved to all orders in bias voltage. If we want to treat the displacement current more accurately such as nonlinear terms in current operator, nonlinear displacement operator should be included. This is a very complicated issue and will be treated in a future publication.

3. Summary

To summarize, we have developed a phenomenological theory for the displacement current operator in the ac regime. With the inclusion of displacement current operator, the frequency dependent noise power under dc bias is conserved and the finite frequency equilibrium fluctuation–dissipation theorem is now consistent with the current conserving dynamic conductance.

Acknowledgments

This work was financially supported the National Natural Science Foundation of China (Grant No. 11374246 and 11404273), the Research Grant Council (Grant No. 17311116), and the UGC (Contract No. AoE/P-04/08) of the Government of HKSAR.

Appendix

There are several relations that we will prove in this supplemental material. It turns out that it is much easier to use NEGF instead of SMT. We will use the following relation to relate G^r and SMT. Decomposing the linewidth function Γ_α using its eigenstate $|W_{\alpha m}\rangle$ where m labels the m th transmission channel, we have $\Gamma_\alpha = \sum_m |W_{\alpha m}\rangle \langle W_{\alpha m}|$ [17]. The wavefunctions $|\psi_{\alpha m}^{(\text{out})}\rangle$ and $|\psi_{\alpha m}^{(\text{in})}\rangle$ are defined as

$$|\psi_{\alpha m}^{(\text{out})}\rangle = \sqrt{v_{\alpha m}} G^r |W_{\alpha m}\rangle, \quad (44)$$

and

$$\langle \psi_{\alpha m}^{(\text{in})} | = \sqrt{v_{\alpha m}} \langle W_{\alpha m} | G^r. \quad (45)$$

It is easy to see that the following relations hold

$$\sum_{\alpha m} |\psi_{\alpha m}^{(\text{in})}\rangle \langle \psi_{\alpha m}^{(\text{in})}| = \sum_{\alpha m} |\psi_{\alpha m}^{(\text{out})}\rangle \langle \psi_{\alpha m}^{(\text{out})}|, \quad (46)$$

and

$$|\psi_{\alpha m}^{(\text{in})}(B)\rangle \langle \psi_{\alpha m}^{(\text{in})}(B)| = [|\psi_{\alpha m}^{(\text{out})}(-B)\rangle \langle \psi_{\alpha m}^{(\text{out})}(-B)|]^T, \quad (47)$$

where B is the magnetic field.

To make the notation simple, we just consider one transmission channel in the following derivation. With the help of the Fisher–Lee relation $s_{\alpha\beta}(E) = -\delta_{\alpha\beta} + i\langle W_\alpha | G^r(E) | W_\beta \rangle$, we will first prove equation (20),

$$\int dx [n_{\beta\gamma}(E, \omega, x)] = \frac{i}{\omega} \sum_\alpha A_{\beta\gamma}(\alpha, E, \bar{E}). \quad (48)$$

On the one hand, with the help of definitions in equations (44) and (45), we find

$$\begin{aligned} \int dx [n_{\beta\gamma}(E, \omega, x)] &= \frac{1}{\sqrt{v_\beta v_\gamma}} \text{Tr}[|\psi_\gamma^{\text{out}}(\bar{E})\rangle \langle \psi_\beta^{\text{out}}(E)|] \\ &= \text{Tr}[\bar{G}^r |W_\gamma\rangle \langle W_\beta| G^a] = \langle W_\beta | G^a \bar{G}^r | W_\gamma \rangle, \end{aligned} \quad (49)$$

where we have used the notation $\bar{G}^r = G^r(\bar{E})$. On the other hand, we can express the $A_{\beta\gamma}(\alpha, E, \bar{E})$ in terms of NEGF using the Fisher–Lee relation,

$$\begin{aligned} \frac{i}{\omega} \sum_\alpha A_{\beta\gamma}(\alpha, E, \bar{E}) &= \frac{i}{\omega} \sum_\alpha [\delta_{\alpha\beta} \delta_{\alpha\gamma} - s_{\alpha\beta}^\dagger(E) s_{\alpha\gamma}(\bar{E})] \\ &= \frac{i}{\omega} \sum_\alpha [\delta_{\alpha\beta} \delta_{\alpha\gamma} + (\delta_{\alpha\beta} + i\langle W_\beta | G^a | W_\alpha \rangle)(-\delta_{\alpha\gamma} + i\langle W_\alpha | \bar{G}^r | W_\gamma \rangle)] \\ &= \frac{i}{\omega} \langle W_\beta | i\bar{G}^r - iG^a - G^a \Gamma \bar{G}^r | W_\gamma \rangle = \langle W_\beta | G^a \bar{G}^r | W_\gamma \rangle, \end{aligned}$$

where we have used $i(\bar{G}^r - G^a) - G^a \Gamma \bar{G}^r = -i\omega G^a \bar{G}^r$ and $\Gamma = \sum_\alpha \Gamma_\alpha$ and therefore equation (20) is proved.

To show $S_{\text{eq}, \alpha\beta}^{(2)}(\omega) = 0$, we will first prove the following relation,

$$\begin{aligned} &\int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} s_{\alpha\gamma}^\dagger(E) s_{\alpha\delta}(\bar{E}) \text{Tr} \left[\frac{d\bar{n}_\beta^*(\omega)}{dE} \mathbf{u}_{\delta\gamma}^*(\omega) \right] \\ &= \int dx dx' g^*(\omega, x, x') \frac{d\bar{n}_\beta^*(\omega, x)}{dE} \frac{d\bar{n}_\alpha(\omega, x')}{dE}. \end{aligned} \quad (50)$$

To do that, we express $s_{\alpha\gamma}^\dagger(E) s_{\alpha\delta}(\bar{E})$ in terms of NEGF

$$s_{\alpha\gamma}^\dagger(E) s_{\alpha\delta}(\bar{E}) = \delta_{\alpha\gamma} \delta_{\alpha\delta} + \langle W_\gamma | iG^a \delta_{\alpha\delta} - i\bar{G}^r \delta_{\alpha\gamma} + G^a \Gamma_\alpha \bar{G}^r | W_\delta \rangle. \quad (51)$$

Then from equations (19), (23), (26) and (27) we have

$$\frac{d\bar{n}_\beta^*(\omega, x)}{dE} = \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} [\bar{G}^a \Gamma_\beta G^r]_{xx}, \tag{52}$$

and

$$u_{\delta\gamma}^*(\omega, x) = \int dx' g^*(\omega, x, x') [G^r | W_\gamma] \langle W_\delta | \bar{G}^a \rangle_{x'x'}. \tag{53}$$

Thus

$$\begin{aligned} \text{Tr} \left[\frac{d\bar{n}_\beta^*(\omega)}{dE} u_{\delta\gamma}^*(\omega) \right] &= \int dx dx' \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \\ &\times [\bar{G}^a \Gamma_\beta G^r]_{xx} g^*(\omega, x, x') [G^r | W_\gamma] \langle W_\delta | \bar{G}^a \rangle_{x'x'}. \end{aligned} \tag{54}$$

Combine with equations (51) and (54), we obtain

$$\begin{aligned} &\int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} s_{\alpha\gamma}^\dagger(E) s_{\alpha\delta}(\bar{E}) \text{Tr} \left[\frac{d\bar{n}_\beta^*(\omega)}{dE} u_{\delta\gamma}^*(\omega) \right] \\ &= \int dx dx' \frac{d\bar{n}_\beta^*(\omega, x)}{dE} g^*(\omega, x, x') \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} \\ &\langle x' | G^r \Gamma_\gamma (G^r \Gamma_\alpha \bar{G}^a - i\bar{G}^r \delta_{\alpha\gamma} + i\bar{G}^a \delta_{\alpha\delta} + G^a \Gamma_\alpha \bar{G}^r) \Gamma_\delta \bar{G}^a | x' \rangle \\ &= \int dx dx' \frac{d\bar{n}_\beta^*(\omega, x)}{dE} g^*(\omega, x, x') \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} [G^a \Gamma_\alpha \bar{G}^r]_{x'x'} \\ &= \int dx dx' g^*(\omega, x, x') \frac{d\bar{n}_\beta^*(\omega, x)}{dE} \frac{d\bar{n}_\alpha(\omega, x')}{dE}, \end{aligned} \tag{55}$$

where we have used the relation $iG^r \Gamma G^a = G^a - G^r$. Similarly, we can prove

$$\begin{aligned} &\int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} s_{\beta\delta}^\dagger(\bar{E}) s_{\beta\gamma}(E) \text{Tr} \left[\frac{d\bar{n}_\alpha(\omega)}{dE} u_{\gamma\delta}(\omega) \right] \\ &= \int dx dx' g(\omega, x, x') \frac{d\bar{n}_\alpha(\omega, x)}{dE} \frac{d\bar{n}_\beta^*(\omega, x')}{dE}. \end{aligned} \tag{56}$$

Next we will prove that

$$\begin{aligned} &\omega^2 \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} \text{Tr} \left[\frac{d\bar{n}_\beta^*(\omega)}{dE} u_{\delta\gamma}^*(\omega) \right] \text{Tr} \left[\frac{d\bar{n}_\alpha(\omega)}{dE} u_{\gamma\delta}(\omega) \right] \\ &= \omega \int dx dx' dx'' dx''' \frac{d\bar{n}_\alpha(\omega, x)}{dE} \frac{d\bar{n}_\beta^*(\omega, x'')}{dE} g(\omega, x, x') \\ &\times g^*(\omega, x', x''') [-i\Pi(\omega, x', x'') + i\Pi^*(\omega, x''', x')], \end{aligned} \tag{57}$$

where $\Pi(\omega, x, x')$ is the Lindhard function (in terms of Green's function, for details see equations (19) to (21) in [9]) defined as

$$\Pi(\omega, x, x') = i \int \frac{dE}{2\pi} [(f - \bar{f}) \bar{G}_{xx'}^r G_{x'x}^a + \bar{f} \bar{G}_{xx'}^a G_{x'x}^r - f \bar{G}_{xx'}^r G_{x'x}^r]. \tag{58}$$

Using equation (54), we have

$$\begin{aligned} &\omega^2 \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} \text{Tr} \left[\frac{d\bar{n}_\beta^*(\omega)}{dE} u_{\delta\gamma}^*(\omega) \right] \text{Tr} \left[\frac{d\bar{n}_\alpha(\omega)}{dE} u_{\gamma\delta}(\omega) \right] \\ &= \omega^2 \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \sum_{\gamma\delta} \int dx dx' g(\omega, x, x') \frac{d\bar{n}_\alpha(\omega, x)}{dE} \\ &\times [\bar{G}^r | W_\delta] \langle W_\gamma | G^a \rangle_{x'x'} \int dx'' dx''' g^*(\omega, x'', x''') \frac{d\bar{n}_\beta^*(\omega, x'')}{dE} \\ &\times [G^r | W_\gamma] \langle W_\delta | \bar{G}^a \rangle_{x''x'''} = \omega^2 \int dx dx' dx'' dx''' \\ &\times g(\omega, x, x') g^*(\omega, x'', x''') \frac{d\bar{n}_\alpha(\omega, x)}{dE} \frac{d\bar{n}_\beta^*(\omega, x'')}{dE} \\ &\times \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} [G^r \Gamma G^a]_{x''x'''} [\bar{G}^r \Gamma \bar{G}^a]_{x'x''}. \end{aligned} \tag{59}$$

It is easy to see

$$\begin{aligned}
& \int \frac{dE}{2\pi} (f - \bar{f}) [(G^r \Gamma G^a)_{x''x'} (\bar{G}^r \Gamma \bar{G}^a)_{x'x''}] \\
&= \int \frac{dE}{2\pi} (f - \bar{f}) [i(G^r - G^a)]_{x''x'} [i(\bar{G}^r - \bar{G}^a)]_{x'x''} \\
&= i[-\Pi(\omega, x', x'') + \Pi^*(\omega, x'', x')].
\end{aligned} \tag{60}$$

Finally we arrive at

$$\begin{aligned}
S_{\text{eq},\alpha\beta}^{(2)}(\omega) &= i\omega \int dx dx' g^*(\omega, x, x') \frac{d\bar{n}_\beta^*(\omega, x)}{dE} \frac{d\bar{n}_\alpha(\omega, x')}{dE} \\
&\quad - i\omega \int dx dx' g(\omega, x, x') \frac{d\bar{n}_\alpha(\omega, x)}{dE} \frac{d\bar{n}_\beta^*(\omega, x')}{dE} \\
&\quad - i\omega \int dx dx' dx'' dx''' \frac{d\bar{n}_\alpha(\omega, x)}{dE} \frac{d\bar{n}_\beta^*(\omega, x'')}{dE} g(\omega, x, x''') \\
&\quad \times g^*(\omega, x''', x''') [\Pi(\omega, x', x''') - \Pi^*(\omega, x''', x')].
\end{aligned} \tag{61}$$

Note that the characteristic potential u_α is defined as

$$\begin{aligned}
u_\alpha(x) &= \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} u_{\alpha\alpha}(x) \\
&= \int \frac{dE}{2\pi} \frac{f - \bar{f}}{\omega} \int dx' g(\omega, x, x') n_{\alpha\alpha}(x') \\
&= \int dx' g(\omega, x, x') \frac{dn_\alpha(x')}{dE}.
\end{aligned} \tag{62}$$

In general all the quantities in equations (61) and (62) are defined in the presence of magnetic field B . We now change the magnetic field from B to $-B$ and combine with the reciprocity relation, we can rewrite $S_{\text{eq},\alpha\beta}^{(2)}(\omega)$ as follows

$$\begin{aligned}
S_{\text{eq},\alpha\beta}^{(2)}(\omega) &= i\omega \text{Tr} \left[u_\beta^*(-B) \frac{dn_\alpha(-B)}{dE} - u_\alpha(-B) \frac{dn_\beta^*(-B)}{dE} \right] \\
&\quad - u_\beta^*(-B) \Pi(\omega, -B) u_\alpha(-B) + u_\alpha(-B) \Pi^*(\omega, -B) u_\beta^*(-B) \\
&= -\frac{i\omega}{4\pi} \text{Tr} [u_\beta^*(-B) \nabla^2 u_\alpha(-B) - u_\alpha(-B) \nabla^2 u_\beta^*(-B)] \\
&= \frac{i\omega}{4\pi} \int_\Omega ds \cdot [u_\alpha(-B) \nabla u_\beta^*(-B) - u_\beta^*(-B) \nabla u_\alpha(-B)],
\end{aligned}$$

where we have used equation (29) and Ω is the boundary of the scattering region. Since deep inside the leads, or at the boundary of the scattering region, the strength of the electric field is zero, we can conclude that $\nabla u_\alpha|_\Omega = 0$. Thus

$$\begin{aligned}
S_{\text{eq},\alpha\beta}^{(2)}(\omega) &= \frac{i\omega}{4\pi} \int_\Omega ds \cdot [u_\alpha(-B) \nabla u_\beta^*(-B) \\
&\quad - u_\beta^*(-B) \nabla u_\alpha(-B)] = 0.
\end{aligned} \tag{63}$$

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