Nonequilibrium Fluctuation-Dissipation Theorems for Interacting Quantum Transport

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We study non-equilibrium (NE) fluctuation-dissipation (FD) relations in the context of quantum thermoelectric transport through a two-terminal nanodevice, in the steady-state and with interaction. The FD relations for the one- and two-particle correlation functions are derived. Numerical applications, using self-consistent NE Green’s functions calculations, are given for electron-phonon interaction in the central region. We find that the FD relations for the one-particle correlation function are strongly dependent on both the NE conditions and the interactions, while they are much less dependent on the interactions for the two-particle correlation. This suggests interesting applications for single-molecule and other nanoscale transport experiments: the two-particle correlation functions, obtained from noise and transport measurement, provide information about the gradients of chemical potential and temperature, and other properties of the system.

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Quantum systems can be driven far from equilibrium by time-dependent perturbation or by coupling to reservoirs at different chemical potentials or temperatures. In the latter case, the system is “open” and particle- or energy-currents flow throughout the system. Such processes take place in different contexts, ranging from nanoscale quantum transport to chemical reactions. The recent developments in modern techniques of microscopic manipulation and nanotechnologies enable us to build functional nanoscale systems. Fluctuations in such systems can nowadays be measured at the single-electron level [1, 2]. At equilibrium, small fluctuations satisfy a universal relation known as the fluctuation-dissipation (FD) theorem [3–5]. The FD relation connects spontaneous fluctuations to the linear response, for both classical and quantum systems.

The search for similar relations for systems driven far from equilibrium has been an active area of research for many decades. A major advance had taken place with the derivation of exact fluctuation relations which hold for classical and quantum systems at non-equilibrium (NE) [6–9]. For quantum systems, fluctuations have also been studied in the context of quantum heat conduction and full counting statistics [10–13]. Another route is to consider the equilibrium relations with effective and local thermodynamical variables (temperature, chemical potential) dependent on the NE conditions [19, 20].

In this paper, we focus on the generalisation of FD relations to NE conditions in the presence of both charge and heat transport, with a strong emphasis on the effects of interactions between particles on such relations. In particular, we derive the NE FD relations for 1-particle correlation functions (the electronic Green’s functions GFs) and for 2-particle correlation functions (the charge-charge (CC) and current-current (JJ) correlation and response functions). We calculate the Kubo-Martin-Schwinger (KMS) and FD relations for a model system connected to two reservoirs in the presence of an applied bias and a temperature gradient, in the NE steady-state.

We show that the FD theorem for the 1-particle correlation functions is strongly dependent on both the NE conditions and the interaction between particles. While the FD relations for the 2-particle correlation functions are much less dependent on the interaction. Such 2-particle quantities are accessible experimentally by noise and transport measurements. Hence one could determine properties of the system such as the effective temperature, the gradients of temperature and chemical potential, the strength of the coupling to the leads, and deviations from electron-hole symmetry.

Equilibrium FD theorems.— At equilibrium, the FD theorem arises from the fact that the time evolution operator $e^{-iHt}$ bears a strong formal similarity to the weighting factor $e^{-\beta H}$ that occurs in the statistical averages by identifying $t \equiv -i\beta$ (with $\beta = 1/kT$). The key relation is that, for any two operators $A$ and $B$, one has

$$\langle A(t - i\beta)B(t') \rangle = \langle B(t')A(t) \rangle.$$

We can define the quantity $X_{AB}^{\pm} = \langle A(1)B(2) \rangle$ and $X_{AB}^{\pm} = \pm \langle B(2)A(1) \rangle$, with the minus (plus) sign for $A, B$ being fermion (boson) operators. At equilibrium, the quantities depend only on the time difference, and after Fourier transform (FT), we write the general FD theorem for $X_{AB}^{\pm}(\omega)$ as

$$X_{AB}^{\pm} = \left[ \frac{r_{AB}(\omega) + 1}{r_{AB}(\omega) - 1} \right] (X_{AB}^{\pm} - X_{AB}^{\mp}),$$

with the ratio $r_{AB}(\omega)$ obtained from the KMS relation at equilibrium $r_{AB}(\omega) = X_{AB}^{\pm}/X_{AB}^{\mp} = e^{\beta\omega}$ with the minus sign for fermion operators and $\omega = \omega - \mu^c$ for (grand-)canonical average (with the equilibrium Fermi level $\mu^c$), and with the plus sign for boson operators ($\omega = \omega$). One recovers the conventional FD relations from Eq. (1). For boson operators, the usual relation between commutator and anticommutator is

$$\langle [A, B] \rangle_\omega = \coth (\beta\omega/2) \langle [A, B] \rangle_\omega.$$
with \((\ldots)_{\omega}\) being the FT of \((\ldots)(t-t')\). For electron Green's functions, \(iG^{>}(1,2) = X_{AB}^{>}(1,2)\) with \(A(1) = \Psi(1)\) and \(B(2) = \Psi(2)\), and we recover the usual relation \(G^{K}(\omega) = \tanh(\beta \omega/2) (G^{>} - G^{<})(\omega)\) by identifying \(G^{K} = G^{>} + G^{<} = i\langle \Psi(1), \Psi(2)\rangle\) and \(G^{r} - G^{a} = G^{>} - G^{−} = i\langle \Psi(1), \Psi(2)\rangle\) [21].

**NE steady-state transport.**—The above KMS and FD relations however do not hold in NE conditions, even in the steady state which can be seen as a pseudo-equilibrium state [22–26]. We now extend the FD relations to NE steady-state transport. We consider the single impurity model connected to two non-interacting Fermi seas. The left \((L)\) and right \((R)\) leads are at their own equilibrium, with a Fermi distribution \(f_{\alpha}(\omega)\) defined by their respective chemical potentials \(\mu_{\alpha}\) and temperatures \(T_{\alpha}\) \((\alpha = L,R)\). The central region connected to the leads contain interaction characterized by a self-energy \(\Sigma_{\text{int}}(\omega)\) [27]. Furthermore the specific model used for the leads does not need to be specified, as long as the leads can be described by an embedding self-energy \(\Sigma_{\alpha}(\omega)\) in the electron GF of the central region. Our results for the FD theorem are general with respect to both the leads and the interaction self-energies.

**FD relations for the 1-particle correlation functions.**—In the absence of interaction in the central region, we use the properties of the GFs in the central region, \(G_{\alpha}^{>}(\omega) = G_{0}^{>}(\omega)(\Sigma_{\alpha}^{>}(\omega) + \Sigma_{\alpha}^{<}(\omega))G_{0}^{<}(\omega)\), to show that they follow a pseudo-equilibrium relation [30]: \(G_{\alpha}^{>}(\omega) = -f^{\text{NE}}(\omega)(G_{L}^{>} - G_{R}^{<}))(\omega)\), where the NE distribution \(f^{\text{NE}} = f^{\text{NE}}(\omega) - 1\) is defined by \(f^{\text{NE}}(\omega) = (\Gamma_{L}(\omega)f_{L}(\omega) + \Gamma_{R}(\omega)f_{R}(\omega))/\Gamma\) and \(\Gamma = \Gamma_{L} + \Gamma_{R}\) with \(\Gamma_{\alpha}(\omega) = i\langle \Sigma_{\alpha}^{<}(\omega)\Sigma_{\alpha}^{<}(\omega)\rangle\). We determine the FD ratio (FDr) from Eq. [4] as \(\text{FD}_{\text{r}}[G_{\alpha}] = (G_{L}^{>} + G_{R}^{<})/(G_{L}^{>} - G_{R}^{<}) = 1 - 2f^{\text{NE}}(\omega)\).

For symmetric coupling to the leads, \(\Gamma_{L} = \Gamma_{R}\) and \(\mu_{L,R} = \mu^{eq} \pm V/2\), we find the following expression [31]:

\[
\text{FD}_{\text{r}}[G_{\alpha}] = \frac{\sinh(\beta \omega)}{\cosh(\beta \omega) + \cosh(\beta V/2)},
\]

and for the KMS ratio \(r_{AB}\):

\[
\frac{G_{\alpha}^{<}}{G_{0}^{<}} = \frac{e^{-\beta \omega} + \cosh(\beta V/2)}{e^{\beta \omega} + \cosh(\beta V/2)}.\]

At equilibrium \((V = 0)\), we recover the usual results \(G_{\alpha}^{>}/G_{0}^{>} = -e^{-\beta \omega}\) and \(\text{FD}_{\text{r}}[G_{\alpha}] = \tanh(\beta \omega/2)\).

For asymmetric contacts and potential drops \(\mu_{\alpha} = \mu^{eq} + \eta_{\alpha}V\) (with \(\eta_{L} - \eta_{R} = 1\)) we find [32]:

\[
\text{FDr} = \frac{\sinh(\beta(\omega - \eta V)) - (\Gamma_{L} - \Gamma_{R}) \sinh(\beta V/2)}{\cosh(\beta(\omega - \eta V)) + \cosh(\beta V/2)},
\]

with \(\eta = (\eta_{L} + \eta_{R})/2\) and \(\Gamma = \Gamma_{L} + \Gamma_{R}\).

In the presence of interaction in the central region, with a self-energy \(\Sigma_{\text{int}}(\omega)\), we use again the properties of the NE GF to find that

\[
\frac{G_{\alpha}^{<}}{G_{\alpha}^{>}} = \frac{\Sigma_{L,R}^{<} + \Sigma_{L,R}^{<}}{\Sigma_{L,R}^{<} + \Sigma_{\text{int}}} = \frac{f_{0}^{\text{NE}} - i\Sigma_{\text{int}}^{<}}{f_{0}^{\text{NE}} - 1 - i\Sigma_{\text{int}}^{<}}\]

From this ratio, we define a NE distribution function \(f^{\text{NE}}(\omega) = [1 - G^{<}/G^{>}^{-1}]\) which permits us to define the pseudo-equilibrium relation \(G^{<} = -f^{\text{NE}}(G^{r} - G^{a})\). It is given by

\[
f^{\text{NE}}(\omega) = \frac{f_{0}^{\text{NE}}(\omega) - i\Sigma_{\text{int}}^{<}(\omega)/\Gamma}{1 + i(\Sigma_{\text{int}}^{<}(\omega)/\Gamma)}.
\]

There is no a priori reason for \(f^{\text{NE}}\) to be equal to the non-interacting distribution \(f_{0}^{\text{NE}}\). From Eq. [7], we derive the FDr \((1 - 2f^{\text{NE}})\) for the interacting GFs

\[
\text{FDr}[G] = \frac{\text{FDr}[G_{0}] + i(\Sigma_{\text{int}}^{<} + \Sigma_{\text{int}}^{<})/\Gamma}{1 + i(\Sigma_{\text{int}}^{<} - \Sigma_{\text{int}}^{<})/\Gamma}.
\]

The NE FD relations, Eqs. [38], derived for the one-particle correlations are less universal than the equilibrium relation, since they depend on both the set-up that drives the system out of equilibrium and on the MB interaction, as expected. However the NE FD relations are universal, with respect to the interaction, in the same sense that the GFs have an universal expression via the use of the interaction self-energies.

We now provide a numerical application for a specific choice of interaction. We consider a model system with electron-phonon (e-ph) interaction for which we calculate the full NE properties using the NE GF Keldysh formalism [31–33]. The Hamiltonian for the central region is \(H_{C} = \varepsilon_{0}d_{L}d_{L} + \omega_{0}\alpha_{l} + \gamma_{l}^{a}d_{L}^{a}d_{L}^{a}\), where \(d_{L}^{a}\) creates (annihilates) an electron in the level \(\varepsilon_{0}\), which is coupled to the vibration mode of energy \(\omega_{0}\) via the coupling constant \(\gamma_{l}\). The leads are represented by one-dimensional tight-binding chains and \(t_{0L,R}\) are the hopping integrals to the central region [36–37]. The many-body (MB) e-ph interaction self-energies \(\Sigma_{\text{int}}\) are treated at the self-consistently Born approximation level [31–33].

We have performed calculations for a wide range of parameters found in [37]. We consider symmetric \((t_{0L} = t_{0R})\) and asymmetric \((t_{0L} \neq t_{0R})\) coupling to the leads, different strengths of coupling \(t_{0L}\), transport regimes (off-resonant \(\varepsilon_{0} \gg \mu^{eq}\), and resonant \(\varepsilon_{0} \sim \mu^{eq}\)), e-ph coupling strengths, biases \(V\) with symmetric and asymmetric potential drops at the contacts, and temperatures \(T_{\alpha}\) and \(T_{\phi}\). All calculations [37] corroborate the conclusions we find for the behaviour of the NE FD ratios that we present below for specific sets of parameters.

Figure 1 shows the FD ratio for the GF for the off-resonant transport regime, in both the presence and the absence of interaction. For zero and very low bias, the FDr follows the equilibrium limit \(\beta \omega/2\) expression as expected. For the non-interacting case, the FDr ratio follows Eq. [3]. One can clearly see that the presence of interaction strongly modifies the FDr. The effects are stronger for larger \(V\) when the bias window include a substantial spectral weight of the self-energy \(\Sigma_{\text{int}}^{<}\). This is the regime when the single-(quasi)particle representation for quantum transport breaks down [33]. At large bias, we can...
obtain negative values of the FDr. This is when the NE MB effects are not negligible and induce strong modifications of the NE distribution $f^{\text{NE}}$. In that case $f^{\text{NE}} > 0.5$ for $\omega \geq 0$ (see inset in Fig. 1). Such a behaviour never occurs in the resonant transport regime (with symmetric coupling to the leads and without Hartree-like self-energy) when the system always presents electron-hole symmetry [37]. These results show that the NE FD theorem for the GF is strongly dependent on the NE conditions as well as on the MB effects. However the NE GF are not directly accessible experimentally as are the electronic current and charge for which the dependence on both the NE and MB effects has been shown in [35, 59].

**FD relations for the 2-particle correlation functions.** — We now calculate the FD relations for the JJ and CC correlation and response functions, far from equilibrium, and compare such relations with those obtained for the GFs. By definition (1), the fluctuation correlation function (noise) is $S_{\alpha\beta}^{X}(t, t') = \frac{1}{2}\left\{ \delta X_{\alpha}(t), \delta X_{\beta}(t') \right\}$ where $\delta X_{\alpha}(t) = X_{\alpha}(t) - \langle X_{\alpha} \rangle$. The response function is $R_{\alpha\beta}^{X}(t, t') = \langle [X_{\alpha}(t), X_{\beta}(t')] \rangle$. For the current flowing at the $\alpha = L, R$ contact: $X_{\alpha} = J_{\alpha}$ and $\langle J_{\alpha}(t) \rangle = e/\hbar \text{Tr}_{\alpha} \left[ (SG)_{\alpha}(t, t) - (GS^\dagger)_{\alpha}(t, t) \right]$. For the charge in the central region: $X_{C} = n_{C}$ and $\langle n_{C}(t) \rangle = e \text{Tr}_{\alpha} \left[ -iG_{\alpha}(t, t) \right]$. The total noise $S^{I}(\omega)$ and response function $R^{I}(\omega)$ are defined from the symmetrized current $J = (J_{L} - J_{R})/2$.

In the steady state, all quantities depend only on the difference $t - t'$ and, after FT, we obtain the relation $2S^{I}(\omega) = \langle xx \rangle_{-} \pm \langle xx \rangle_{+}$ with $\langle xx \rangle_{-} = (jj)_{-}^\dagger$ for the current, or $\langle n_{C}n_{C} \rangle_{-}^\pm$ for the charge [39, 40]. The two-particle correlation functions are bosonic. At equilibrium they follow the relation $2S^{I}(\omega) = \coth (\beta \omega/2) R^{I}(\omega)$ [35].

We now compute the two-particle correlation functions and the FD relations using our model NEGF calculations with $e$-ph interaction. We concentrate below on the inverse of the NE FD ratio $1/FDr = R^{I}(\omega)/2S^{I}(\omega)$ for JJ and CC correlation functions. This allows us to avoid the divergence of the coth-like function at $\omega = 0$, and allows for a direct comparison with the FDr of the GFs (function $\tanh \omega/2$ at equilibrium). Figure 2 shows the inverse FDr of the JJ correlation functions for the off-resonant regime (same parameters as in Fig. 1) (for the resonant regime see [37]). The inverse of FDr for the JJ correlation functions does not have the same behaviour as the FDr of the GFs [37], although it follows the same $\tanh \beta \omega/2$ behaviour at very small applied bias, as expected. Increasing the bias, seems to correspond to an effective increase of the temperature. However the FDr[JJ] is never well represented by an $\tanh \beta \omega/2$ function (with an effective local temperature $kT_{\text{eff}} = 1/\beta \hbar$) beyond the linear regime [37]. More importantly, the NE FD ratio for the JJ correlations is much less dependent on the interaction than FDr[GF]. This is a very interesting property, useful for experiments as we explain below.

Figure 3 shows the inverse FDr of the CC correlation functions in the off-resonant regime (same parameters as in Fig. 1). We observe again that the interaction effects are less dominant in FDr[CC] than in FDr[GF], except for large bias. Furthermore we find that FDr[CC] $\neq$ FDr[JJ] [37]. The reasons why the FDr ratios for the JJ and the CC correlations and GFs are all different can be understood from the NE density matrix (including both NE and MB effects) introduced by Hershfield as
\( \rho \equiv e^{-\beta(H-Y)} \) \cite{22}. The \( Y \) operator is constructed from an iterative scheme for the equation of motion of an initial \( Y_0 \) operator. In the case of a two-terminal device, the initial operator is \( Y_0 = \mu_L N_L + \mu_R N_L \) with the left and right chemical potentials \( \mu_{L,R} \) and particle number operators \( N_{L,R} \). The key relation leading the FD theorems becomes

\[
(A(t - i\beta)B(t')) = (e^{-\beta V} B(t')e^{\beta V} A(t)).
\]

The usual equilibrium FD relations break down at NE and additional contributions arise from the expansion

\[
e^{-\beta V} Be^{\beta V} = B + [-\beta Y, B] + \ldots \]

\cite{22,40}. For the GFs of the central region, the fermion operator \( \hat{B} \) is \( d \) \( d \) or \( d^\dagger d \) \( d^\dagger d \) where \( d^\dagger \) \( d^\dagger \) creates (annihilates) an electron in the lead \( \alpha \). Therefore there is no obvious reason for the two FD ratios to be identical, especially in the presence of interaction. Furthermore, with the JJ and CC correlations, one deals with an higher order product than for the GFs and the expansion of \( e^{-\beta V} Be^{\beta V} \) contains higher order powers in terms of the interaction coupling parameters (in case our case, in terms of \( \gamma^2 \gamma^0 \) in comparison to the series expansion for the GFs. Therefore, for weak to intermediate interaction strengths, we expect less effect from the interaction in the FDr of the JJ and CC correlations than in FDr[G] as shown above.

With temperature gradient.— So far we have considered systems with a unique temperature. We also consider cases where there is a temperature gradient between the \( L \) and \( R \) lead. The derivations follow the same line as previously, and we find the NE FD ratio for the symmetric non-interacting case (in the presence of both a potential and temperature gradients between the two leads):

\[
\text{FDr}[G_0] = \frac{(2 \sinh \beta \omega)}{(2 \cosh \beta \omega + (u^{-\beta L} + u^{-\beta R}) \times \cosh \Delta \beta \omega/2 + (u^{-\beta L} - u^{-\beta R}) \sinh \Delta \beta \omega/2)},
\]

with \( u = e^{V/2} \), \( \tilde{\beta} = (\beta_L + \beta_R)/2 \) and \( \Delta \beta = \beta_L - \beta_R \). Clearly, at zero bias, the gradient \( \Delta \beta \) plays the same role as the bias \( V \) in Eq. \([3]\) with an effective temperature \( T_{\text{eff}} \) defined from \( \beta \) as \( T_{\text{eff}} = T_L T_R/(T_L + T_R) \). The calculations we have performed in the presence of both temperature gradient and applied bias show similar behaviours as described above \cite{37}. Now we have two “forces” driving the system out of equilibrium, \( \Delta \mu \) and \( \Delta \beta \), and the FD relations (at low bias) are governed by the effective temperature \( 1/\beta \).

Discussion.— We have derived FD relations for one-particle and two-particle correlation functions in the context of quantum transport through a two-terminal device in the steady state regime. We have also provided numerical application of our derivation for the case of a single impurity model in the presence of e-ph interaction. Our calculations are mostly relevant for e-ph interacting systems, but are not limited only to these processes. The main conclusion of our work is that the FD relations for the GFs are strongly dependent both on the ‘forces’ (\( \Delta \mu \) and/or \( \Delta \beta \)) driving the system out of equilibrium and on the interaction, while the FD relations for the current–current correlation functions are much less dependent on the interaction. However the JJ FD relations cannot be well described by equilibrium relations using an effective local temperature (which would be dependent on the applied ‘forces’).

The weak dependence on interaction of the JJ FD relation implies that the calculated relation for the non-interacting case can serve as a master curve for fitting experimental results. The experimental JJ correlation functions obtained via noise and transport measurement, fitted on the master curve, can provide us with information about the forces (\( \Delta \mu \) and/or \( \Delta \beta \)) and effective temperature in the central region. These are crucial quantities to know in single-molecule nanodevice experiments. Furthermore, a strong departure from the master curve could indicate a breakdown of the major hypothesis of our model, i.e. the interactions are not located only in the central region, or there are more than two energy/particle reservoirs connected to the central region.

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[33] Equality occurs only in special cases for which $\Sigma^{\text{int}}$ follows the statistics $\Sigma^{\text{int}} = -f^{\text{eq}}(\Sigma^{\text{int}} - \Sigma^{\text{tot}})$, but this is generally not true. For e-ph interaction, the lowest order self-energy is given by the Fock diagram: $\Sigma^{\text{int}}(\omega) = \frac{\gamma}{(N_{ph}G^S(\omega + \omega_i) + (N_{ph} + 1)G^S(\omega + \omega_i))}$ [34]. At low temperature $N_{ph} = 0$ and the ratio $\Sigma^{\text{int}}/\Sigma^{\text{tot}} = G_r^S(\omega - \omega_i)/G_r^S(\omega + \omega_i)$ defines a distribution function with the usual relation $\Sigma^{\text{int}}(\omega) = [1 - \Sigma^{\text{int}}/\Sigma^{\text{tot}}]^{-1}$ complete different from $f^{eq}$. At equilibrium, we recover the current (Nyquist-Johnson) noise $S^r(0) = 2kT G_{\text{in}}$ with the linear conductance $2G_{\text{in}} = \lim_{\omega_0 \rightarrow 0} R(\omega)/\omega$ [1].
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