Landauer current and mutual information

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We study quantum evolution of the mutual information of a quantum dot connected to left and right leads initially maintained at chemical potentials $\mu_L$ and $\mu_R$, respectively, within the noninteracting resonant-level model. The full nonequilibrium mixed state density matrix of the whole system is written down exactly, and the mutual information of the dot with respect to the leads is computed. A strong and direct correlation is found between the Landauer current and the mutual information at all times, the steady-state values in particular displaying a quadratic relationship at high temperatures. Strikingly, it is found that one can obtain a maximal mutual information by simply applying a sufficiently large “source-drain” voltage $V_{SD}$ even at high temperatures.

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\textbf{I. INTRODUCTION}

The tunneling current across a quantum dot in a non-interacting electron framework has been studied for some five decades now [1–5] and is widely regarded as well understood because it is amenable to an analytical solution within the powerful nonequilibrium Green function framework \cite{1,6}. Recently developed numerical methods \cite{7–14} have made the study of interacting systems driven away from equilibrium an accessible task as well. Although the notion of entanglement, arguably the most fundamental aspect of “quantum physics,” has been around since the birth of quantum mechanics, it is only in the past decade or so its study in various contexts of physics has become popular \cite{15–18}. Understandably, this has coincided with the development of a whole machinery of mathematical tools to quantify it \cite{19} and simultaneous advances in numerical approaches \cite{20} which allow for a direct utilization of the machinery. It is of great current interest in almost every discipline of physics to explore hitherto unexpected connections to entanglement.

Here we investigate the connection between mutual information and Landauer current in a simple noninteracting resonant-level model. Related recent studies have either restricted themselves to looking at the system as a pure state in order to extract an exact useful relationship with quantum noise \cite{21,22} or have briefly hinted the possibility of calculating entanglement as an aside \cite{23}. Here, with mutual information of the quantum dot with respect to the leads for the full nonequilibrium mixed state as our focus, we derive explicitly how the nonequilibrium density matrix of the system can be expressed as an effective thermal density matrix. This result is in agreement with the general thermal density matrix prescription that was developed formally within a so-called $Y$ operator approach a while back by Hershfield \cite{24}.

We start by recalling how the nonequilibrium current is recovered with the aid of a simple prescription. Employing the methods of Ingo Peschel \cite{25}, we then proceed to obtain the von Neumann entropy of any part of the full system with respect to its bath in terms of a correlation matrix. Introducing the notion of mutual information \cite{26,27} we are then able to calculate and study the total correlation between the dot (which is taken as our system) and the bath (given by the two leads). A strong correlation between the current and the entanglement between the dot and the leads is seen. Surprisingly, the maximal mutual information (MI) of the quantum dot with respect to the leads is attained at steady state by the application of a large “source-drain” voltage, unlike the effect of temperature which tends to cause the mutual information to fall, thus making voltage and temperature not alike in this respect.

\textbf{II. THE MODEL}

We consider the following tunneling Hamiltonian:

$$\mathcal{H} = \mathcal{H}_D + \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_{LD} + \mathcal{H}_{RD}$$

$$\mathcal{H}_D = \epsilon_d \hat{d} \dagger \hat{d}$$

$$\mathcal{H}_{LL(R)} = \sum_{k \in L(R)} \epsilon_k \hat{c}_k ^\dagger \hat{c}_k$$

$$\mathcal{H}_{LD(RD)} = \sum_{k \in L(R)} t_k (\hat{d} \dagger \hat{c}_k + \hat{c}_k ^\dagger \hat{d}),$$

where $\epsilon_d$ is the energy of the isolated quantum dot, $\epsilon_k$ is the energy of the electrode mode $k$, and $t_k$ is the coupling between the the quantum dot and the electrode mode $k$ (with the energy levels and the couplings of both left and right electrodes assumed to be identical). The “wide-band limit” \cite{7,28} with a sharp cutoff at high and low energy values is imposed:

$$J_{L/R} (\epsilon) = \frac{\Gamma_{L/R}}{[1 + e^{A (\epsilon - \frac{\epsilon_d}{2})}][1 + e^{-A (\epsilon + \frac{\epsilon_d}{2})}]}.$$  \hfill (2)

with $\Gamma_L = \Gamma_R = \frac{1}{2}$, $\Gamma = \Gamma_L + \Gamma_R$, $A = 5\Gamma$, and $B = 20\Gamma$. We set $\hbar = 1$, $k_B = 1$, and electronic charge $e = 1$ throughout. With a uniform discretization the couplings are given by $t_k (\epsilon_k) = \sqrt{\frac{\sqrt{A \Delta \epsilon}}{2 \pi}}$. Further, we assume that at time $t = 0$, the left and right leads are separately at thermal equilibrium each at the same temperature $T$ and characterized by chemical potentials $\mu_L$ and $\mu_R$, respectively, with $\mu_L - \mu_R = e V_{SD}$ being the applied external “voltage,” and the tunneling Hamiltonian between the leads suddenly turned on at time $t = 0$. At time $t = 0$, therefore, we have the full system in the following mixed
but separable state:

$$\rho(0) = \rho_L(0) \otimes \rho_R(0) \otimes \rho_D(0),$$  \hspace{1cm} (3)

where the left and right leads are in thermal ensembles,

$$\rho_L(0) = \frac{e^{-\beta (H_L - \mu_L) \sum c_\alpha c_\alpha^\dagger}}{Z_L},$$  \hspace{1cm} (4)

$$\rho_R(0) = \frac{e^{-\beta (H_R - \mu_R) \sum c_\alpha c_\alpha^\dagger}}{Z_R},$$  \hspace{1cm} (5)

and the dot is characterized by an arbitrary population \(n_0\),

$$\rho_D(0) = n_0 d^\dagger d + (1 - n_0) d d^\dagger.$$  \hspace{1cm} (6)

### III. CURRENT

Although the thermodynamic limit of this problem can be solved, in order to study mutual information, we consider a sufficiently large but finite system (whose convergence to thermodynamic limit we verified) with \(N_L = 128, N_R = 128\) sites on the left and right leads respectively. The full hopping matrix can be written explicitly as:

$$T = \begin{pmatrix}
\varepsilon_1 & 0 & \cdots & 0 & 0 & \cdots & 0 & t_1 \\
0 & \varepsilon_2 & \cdots & \cdots & \cdots & \cdots & \cdots & t_2 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
\cdots & \cdots & \varepsilon_N & 0 & \cdots & \cdots & t_{N_L} \\
0 & 0 & \cdots & 0 & \varepsilon_3 & \cdots & \cdots & t_1 \\
0 & 0 & \cdots & \cdots & 0 & \varepsilon_3 & \cdots & t_3 \\
\vdots & \ddots & \ddots & \ddots & \cdots & \cdots & \cdots & \ddots \\
0 & \cdots & \cdots & \cdots & 0 & \cdots & 0 & \varepsilon_{N_R} & t_{N_R} \\
t_1 & t_2 & \cdots & t_{N_L} & t_1 & t_2 & \cdots & t_{N_R} & \varepsilon_d
\end{pmatrix}.$$  \hspace{1cm} (7)

Next, we diagonalize the hopping matrix:

$$\sum_{\alpha=1}^{N} T_{ij} \psi_\alpha(j) = e^{\varepsilon_\alpha} \psi_\alpha(i),$$  \hspace{1cm} (8)

where \(N\) is the total number of sites inclusive of the left and right leads and one dot: \(N = N_L + N_R + 1\). The eigenvalues \(e_\alpha\) are ordered such that \(e_1 \leq e_2 \leq \cdots \leq e_N\). By defining the fermionic operators \(a_\alpha = \sum_{\omega=1}^{N} \psi_\alpha(i) c_i\), the Hamiltonian Eq. (1) becomes \(H = \sum_{\alpha=1}^{N} e_\alpha a_\alpha^\dagger a_\alpha\). The eigenstates of the Hamiltonian can all be written in the form \(|E\rangle = \prod_{\alpha=1}^{N} e_\alpha^{\dagger} a_\alpha|0\rangle\), with \(N_p\) particles, and the energy \(E = \sum_{\alpha=1}^{N} e_\alpha\) is simply given as the sum of the single-particle states occupied. Since every state can be either occupied or not, the total number of distinct eigenstates is \(2^N\).

The left (right) current is given by the change in occupancy of the left (right) electrode:

$$I_{L(R)}(t) = -e \frac{d}{dt} \left( \sum_{i \in L(R)} c_i^\dagger c_i \right),$$  \hspace{1cm} (9)

$$= -\frac{e i}{\hbar} \sum_{i \in L(R)} t_i (d^\dagger c_i - c_i^\dagger d).$$  \hspace{1cm} (10)

The overall current defined as \(I(t) = I_{L(t)} - I_{R(t)}\) can be computed as (Appendix A):

$$I(t) = \sum_{jk} \tilde{t}_j \sum_{\alpha\beta} \text{Im} \left[ e^{i(t \varepsilon_\alpha - \varepsilon_\beta)} \alpha(N) \beta(k) \psi^*_\alpha(j) \psi^*_\beta(k) \psi^*_\beta(k) \psi^*_\beta(k) \right] f_k,$$  \hspace{1cm} (11)

where \(\tilde{t}_j = t_j\) if \(j \in L\) and \(\tilde{t}_j = -t_j\) if \(j \in R\) and where \(f_k\) is the Fermi function \(f(\varepsilon_k - \mu_L)\) for modes on the left lead, the occupancy \(n_0\) for the dot mode.

### IV. NONEQUILIBRIUM DENSITY MATRIX

In the Schrödinger picture, the time evolved density matrix is given by

$$\rho(t) = e^{-iHt/\hbar} \rho(0) e^{iHt/\hbar}.$$  \hspace{1cm} (12)

Since the initial density matrix is of the form \(\rho(0) = \rho_L \otimes \rho_R \otimes \rho_D\), Wick’s theorem holds at \(t = 0\), and therefore (Appendix B) Wick’s theorem must hold at every instant of time, i.e., every higher-order correlator can be written in terms of one-particle correlators:

$$\langle c_{\alpha}^\dagger c_{\alpha}^\dagger c_{\beta} c_{\beta} \rangle = \langle c_{\alpha}^\dagger c_{\alpha} \rangle \langle c_{\beta}^\dagger c_{\beta} \rangle - \langle c_{\alpha}^\dagger c_{\beta} \rangle \langle c_{\alpha}^\dagger c_{\beta} \rangle,$$  \hspace{1cm} (13)

the expectation value of an operator \(A(\rho) = \langle A \rangle(t)\) being defined as usual:

$$\langle A \rangle(t) = \text{Tr}(\rho(t) A).$$

But we know that the density matrix is unique and that if it takes the form

$$\rho(t) = \frac{e^{-\sum_c H_i(t)c^\dagger c}}{Z},$$  \hspace{1cm} (14)

then Wick’s theorem holds. Imposing this form, one can show that (Appendix B) the matrix \(H(t)\) is simply determined by the relation

$$\exp(H(t)) = -C(t) + 1 \frac{C(t)}{C(0)},$$  \hspace{1cm} (15)

in terms of the correlator matrix defined as

$$C_{ij}(t) = \text{Tr}(\rho(t)c_i^\dagger c_j).$$  \hspace{1cm} (16)
V. MUTUAL INFORMATION

We wish to study the entanglement between the dot and the leads. The typical quantity that is used to study the entanglement between a system and its bath is the von Neumann entropy of the reduced density matrix (of either system or bath). However, in our case, this is unsuitable because the overall composite state of dot and leads given by $\rho(t)$ is a mixed state. This implies that the von Neumann entropy of the dot would differ from the von Neumann entropy of the leads, thus making a blind application not amenable to study bipartite entanglement. A simple workaround exists and that is to study mutual information defined as:

$$ S = S_D + S_{LR} - S_{\text{full}}, $$

where $S_D = - \text{Tr}(\rho_D \ln \rho_D)$, $S_{LR} = - \text{Tr}(\rho_{LR} \ln \rho_{LR})$, and $S_{\text{full}} = - \text{Tr}(\rho \ln \rho)$, and the reduced density matrices are defined as usual: $\rho_D = \text{Tr}_{L,R}(\rho)$, $\rho_{LR} = \text{Tr}_D(\rho)$.

The mutual information includes both classical and quantum correlations; however, it is a much studied object of interest in its own right [17,18]. An implicit dependence of other for a range of parameters. We found that at sufficiently

The reduced density matrices themselves can be written as thermal density matrices of the form $\rho_{\text{red}} = \frac{e^{-\sum_i n_i c_i c_i^\dagger}}{Z}$ by the same argument given in the previous section: Wick’s theorem holds within the reduced subspace, and the reduced density matrix is unique, and Wick’s theorem holds for a thermal type of density matrix. Once again the $H$ matrix is related to the correlator matrix $C$ by the formula $\exp(H) = (-C + 1)C^{-1}$, with the crucial difference that the correlator matrix indices run only over the reduced subspace. We now obtain a simple formula for the von Neumann entropy of any subspace $G$:

$$ S_G = - \text{Tr}(\rho_G \ln \rho_G), $$

in terms of the eigenvalues of the correlator matrix within that subspace. With the aid of this general formula the mutual information is easily computed by replacing $G$ with $D$, $LR$, and “full” in Eq. (17). As shown in Appendix C,

$$ S_G = \sum_{\sigma=1}^{N_G} [(1 - C_\sigma) \ln(1 - C_\sigma) - C_\sigma \ln C_\sigma], $$

where $C_\sigma$ are the eigenvalues of the correlator matrix defined within the reduced subspace $G$. Thus the computation of von Neumann entropy has been reduced from a $2^{N_L} \times 2^{N_R}$ eigenvalue problem to a $N_G \times N_G$ eigenvalue problem, where $N_G$ is the number of sites in the subspace under consideration. This can be exploited for numerics and we do. This above formula is general and applicable for the full nonequilibrium state at arbitrary time; a similar formula was obtained for eigenstates [29] and for the nonequilibrium steady state [23].

In our case, the von Neumann entropy of the full density matrix $S_{\text{full}}$ is constant in time, as is evident from the unitary evolution of the density matrix $\rho(t)$ in Eq. (12), which leaves the eigenvalues of $\rho(t)$ invariant. We can write down an expression for $S_{\text{full}}$ in terms of the initial density matrix, similar to Eq. (19), where the eigenvalues $C_\sigma$ are just the population $n_\sigma$ and Fermi functions for the left and right leads as given in Eq. (11).

VI. CURRENT AND MUTUAL INFORMATION

Figure 1 shows the intimate relation between current and mutual information, which is the heart of our finding here. We see that the greater the current the greater the mutual information. In fact, it seems that the underlying mechanism by which one may attain high current is to attempt to make the dot highly entangled with its environment. Conversely, a simple method by which to obtain high-MI states may be simply to maximize current in a quantum-dot-system, one that is well studied and where considerable experimental expertise exists. We verified this direct relationship between current and MI for a series of different parameters ($T$, $eV_{SD}$); only a representative sample is displayed in Fig. 1. A further striking aspect of Fig. 1 is that the maximal MI of the dot ($S \sim 2 \log_2 2$) can be obtained even at high temperatures by the application of a large “source-drain” voltage ($eV_{SD} \gg k_B T$), an observation that could be exploited experimentally for producing maximal MI quantum dots. In order to see if further order exists between current and MI, we studied the steady-state dependence of each other for a range of parameters. We found that at sufficiently

![FIG. 1. (Color online) The intimate relationship between current and mutual information, which is the heart of our finding here.](https://example.com/fig1.png)
It is known that $I_\infty$ in the limit of high temperature has a linear dependence on $(\mu_L - \mu_R)$ ("Ohm’s law"), thus Fig. 2 implies that at high temperature $S_\infty$ has a quadratic dependence on voltage. Our numerical checks show that this quadratic dependence on voltage appears to be true term by term for all orders in Eq. (21), an abstract implication of which is that the spectral function of the correlator matrix is quadratic. This is a remarkable, strange, and nontrivial finding and appears to be not accessible to simple arguments.

VII. CONCLUSIONS AND DISCUSSION

We studied the dynamics of a quantum dot within the noninteracting resonant level model. With Heisenberg time evolution we were able to obtain the exact nonequilibrium density matrix at arbitrary time, which in turn allowed us to study the Landauer current. Working with the notion of mutual information, we obtained a convenient expression by which one can study the nonequilibrium MI between the dot and the leads as a function of time. We found that the current through the system and the MI between the quantum dot and the leads are intimately and directly related. Studying the steady-state mutual information $S_\infty$, we noticed that this quantity has a strong quadratic dependence with respect to the steady-state current $I_\infty$, particularly at high temperatures—this appears to be a strange, nontrivial finding. We also observed that at sufficiently high temperatures, one can find a window of where the MI is linear with respect to the quantum fluctuations in steady-state current, $\nu_\infty$. We envisage that these observations could be useful for future electronics applications: namely design of high-current devices. Also, we speculate that a simple way to generate high MI could be to simply achieve high current in certain systems. Strikingly, it is found to be possible to generate states with maximal MI for the quantum dot even at high temperatures by simply applying a large "source-drain" voltage. Although MI includes both quantum and classical correlation, at very low temperatures, the system gets closer and closer to pure states, in which case MI is exactly 2 times the entanglement entropy; thus, in order to exploit our understanding for the harnessing pure quantum correlations in an experimental setting, low temperatures would be appropriate. Further studies on this would be desirable to clarify and perhaps quantify some of these dependencies and also to consider other kinds of systems to see if these features are universal.

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**APPENDIX A: CURRENT**

In terms of the fermionic operators

\[ a_α = \sum_{i=1}^{N} \psi_α(i)c_i, \]

the Hamiltonian becomes \( \mathcal{H} = \sum_{a=1}^{N} e_a a_α^\dagger a_α \).

Since

\[ \sum_{a=1}^{N} \psi_α^\dagger(j) a_α = \sum_{a=1}^{N} \sum_{i=1}^{N} \psi_α^\dagger(j) \psi_α(i) c_i \]

\[ = \sum_{i=1}^{N} \delta_{i,j} c_i, \]

\[ c_j = \sum_{a=1}^{N} \psi_α^\dagger(j) a_α. \]

We note that for \( j = 1, \ldots, N_L \) these destruction operators refer to the left lead, for \( j = (N_L + 1), \ldots, (N_L + N_R) \) to the right lead, and for \( j = N \) to the dot (\( c_N \equiv d \)).

The time evolution of the Heisenberg operators \( a_α(t) \) can be easily written down,

\[ \dot{a}_α = \frac{i}{\hbar} \left[ a_α, \sum_β e_β a_β^\dagger a_β \right] \]

\[ = \frac{i}{\hbar} e_α a_α. \]

Therefore (with \( \hbar = 1 \)),

\[ a_α(t) = e^{-i\epsilon_α t} a_α(0). \]

Thus, with the help of the relation between the \( c \) and \( a \) operators, the time evolution of all the original operators \( c_j(t) \) is easily obtained.

The left current is given by the change in occupancy of the left electrode:

\[ I_L(t) = -e \frac{d}{dt} \left( \sum_{j \in L} c_j^\dagger c_j \right), \]

\[ = -\frac{e i}{\hbar} \left( \sum_{j \in L} t_j (d_j^\dagger c_j - c_j^\dagger d_j) \right). \]

From Eq. (A5), and from the relation between the \( c \) and \( a \) operators, we can write

\[ \langle c_m^\dagger(t)c_n(t)c_i(t)c_j(t) \rangle = \sum_{αβγ δ} \psi_α(p)\psi_β^\dagger(q)\psi_γ^\dagger(l)\psi_δ(j)a_δ^\dagger(t)a_β(t)a_γ(t)a_δ(t) \]

\[ = \sum_{αβγ δ} \psi_α(p)\psi_β^\dagger(q)e^{i(\epsilon_α-\epsilon_δ)}(a_δ^\dagger(0)a_δ(0)) \]

\[ = \sum_{αβγ δ} e^{i(\epsilon_α-\epsilon_δ)}\psi_α(p)\psi_β^\dagger(q) \]

\[ \times \sum_{kl} \psi_α^\dagger(k)\psi_β(l)(c_k^\dagger(0)c_l(0)). \]

The left current can now be written as (with \( \hbar = 1, e = 1 \)):

\[ I_L(t) = 2 \sum_{j \in L} t_j \sum_{αβ} \text{Im}[e^{i(\epsilon_α-\epsilon_δ)}\psi_α(N)\psi_α^\dagger(j)\psi_β^\dagger(k)\psi_β(l)] \]

\[ \times \langle c_i^\dagger(0)c_j(0) \rangle, \]

where we have used the fact that the dot operator corresponds to the \( N^{th} \) mode in our representation. A similar expression exists for the right current. Therefore, combining the two and defining

\[ \tilde{t}_j = t_j \quad \text{if} \quad j \in L \]

\[ = -t_j \quad \text{if} \quad j \in R, \]

we can compute the overall current,

\[ I(t) = \sum_{j} \tilde{t}_j \sum_{αβ} \text{Im}[e^{i(\epsilon_α-\epsilon_δ)}\psi_α(N)\psi_α^\dagger(j)\psi_β^\dagger(k)\psi_β(l)] \]

\[ \times \langle c_i^\dagger(0)c_j(0) \rangle. \]

Our initial condition is such that

\[ \langle c_i^\dagger(0)c_j(0) \rangle = \delta_{ij} f, \]

where \( f \) is the Fermi function \( f(\epsilon_k - \mu_L) \) for modes on the left lead, the Fermi function \( f(\epsilon_k - \mu_R) \) for modes on the right lead, and the occupancy \( n_0 \) for the dot mode. Thus the summation simplifies for the expression for current.

**APPENDIX B: DETERMINATION OF THE \( H \) MATRIX IN TERMS OF THE CORRELATOR MATRIX \( C \)**

Because of our choice of initial density matrix which is of the form \( ρ(0) = \frac{1}{Z} \sum_{ijk} \rho_{ijk} |ij⟩⟨k⟩ \), Wick’s theorem holds at \( t = 0 \). Therefore,

\[ \langle c_m^\dagger(t)c_n(t)c_i(t)c_j(t) \rangle = \sum_{αβγ δ} \psi_α(n)\psi_β^\dagger(m)\psi_γ^\dagger(l)\psi_δ(j)a_δ^\dagger(t)a_β(t)a_γ(t)a_δ(t) \]

\[ = \sum_{αβγ δ} \psi_α(n)\psi_β^\dagger(m)\psi_γ^\dagger(l)\psi_δ(j)e^{i(\epsilon_α+\epsilon_δ-\epsilon_β-\epsilon_γ)}(a_δ^\dagger(0)a_β(0)a_γ(0)a_δ(0)) \]

\[ = \sum_{αβγ δ} \psi_α(n)\psi_β^\dagger(m)\psi_γ^\dagger(l)\psi_δ(j)e^{i(\epsilon_α+\epsilon_δ-\epsilon_β-\epsilon_γ)}[(a_δ^\dagger(0)a_δ(0))a_β(0)a_γ(0) - (a_δ^\dagger(0)a_δ(0))a_β(0)a_γ(0)] \]

\[ = \langle c_i^\dagger(0)c_j(t) \rangle \langle c_m^\dagger(t)c_n(t) \rangle - \langle c_i^\dagger(0)c_n(t) \rangle \langle c_m^\dagger(t)c_j(t) \rangle, \]

\[ \text{B1} \]
thus showing that Wick's theorem holds at arbitrary time. Therefore, we posit that $\rho(t)$ has the form

$$\rho(t) = \frac{e^{-\sum_i h_i(t)c_i^\dagger c_i}}{Z} \quad (B2)$$

and now calculate the matrix $H_{ij}(t)$. For clarity, we make the time dependence of quantities implicit henceforth. Let $\phi_\sigma(i)$ be the eigenfunctions of $H$ with eigenvalues $h_\sigma$. Then the transformation to new fermion operators $a_\sigma$,

$$a_\sigma = \sum_{i=1}^L \phi_\sigma(i)c_i, \quad (B3)$$

gives

$$\rho(t) = \frac{\exp\left(-\sum_{\sigma=1}^L h_\sigma a_\sigma^\dagger a_\sigma\right)}{\prod_{\sigma=1}^L (1 + e^{h_\sigma})}. \quad (B4)$$

It turns out that the correlator matrix defined as

$$C_{ij} = \text{Tr}(\rho(t)c_i^\dagger c_j) \quad (B5)$$

is also diagonalized by precisely the same eigenfunctions that diagonalize the matrix $H$. This is seen simply as follows:

$$\sum_j C_{ij}\phi_\sigma(j) = \text{Tr}\left(c_i^\dagger \sum_j c_j\phi_\sigma(j)\rho(t)\right)$$

$$= \text{Tr}(c_i^\dagger \text{Tr}(c_\sigma\rho(t)))$$

$$= \text{Tr}\left(\sum_j \phi_\sigma(i)\phi_\sigma(j)\rho(t)\right)$$

$$= \text{Tr}(a_\sigma^\dagger a_\sigma\rho(t))$$

$$= \frac{e^{-h_\sigma}}{1 + e^{-h_\sigma}} \phi_\sigma(j), \quad (B6)$$

where we have used the precise diagonal form of Eq. (B4) to simplify. Thus the matrices $C$ and $H$ share eigenfunctions, and the relationship between their eigenvalues implies that we can write

$$\exp(H) = (-C + 1)C^{-1}, \quad (B7)$$

which completes the procedure for how to obtain the full nonequilibrium density matrix as an effective thermal density matrix.

**APPENDIX C: VON NEUMANN ENTROPY OF A SUBSYSTEM OF THE FULL NONEQUILIBRIUM MIXED-STATE DENSITY MATRIX**

The reduced density matrices themselves can be written as thermal density matrices of the form $\rho_{\text{red}} = \frac{e^{-\sum_i h_i(t)c_i^\dagger c_i}}{Z}$ by the same argument given in the previous section: Wick’s theorem holds within the reduced subspace, and the reduced density matrix is unique, and Wick’s theorem holds for a thermal type of density matrix. Once again the $H$ matrix is related to the correlator matrix $C$ by the formula $\exp(H) = (-C + 1)C^{-1}$, with the crucial difference that the correlator matrix indices run only over the reduced subspace. We now obtain a simple formula for the von Neumann entropy of any subspace $G$:

$$S_G = -\text{Tr}(\rho_G \ln \rho_G), \quad (C1)$$

$$S_G = -\text{Tr}\left[\frac{1}{Z} \exp\left(-\sum_{\sigma=1}^L h_\sigma a_\sigma^\dagger a_\sigma\right) \times \left(\frac{1}{Z} - \sum_{\sigma=1}^L h_\sigma a_\sigma^\dagger a_\sigma\right)\right]$$

$$= \sum_{\sigma=1}^L \ln[1 + \exp(-h_\sigma)]$$

$$+ \sum_{\sigma=1}^L \left[\frac{h_\sigma}{1 + \exp(h_\sigma)}\right]$$

$$= \sum_{\sigma=1}^L \left[\ln[1 + \exp(-h_\sigma)] + \frac{h_\sigma}{1 + \exp(h_\sigma)}\right] \quad (C2)$$

But, we know that

$$\exp(h_\sigma) = \frac{1 - C_\sigma}{C_\sigma}, \quad (C3)$$

where $C_\sigma$ is the corresponding eigenvalue of the correlator matrix in Eq. (B5) defined with the subspace $G$. Therefore,

$$S_G = \sum_{\sigma=1}^L [-\ln(1 - C_\sigma) - C_\sigma \ln C_\sigma]. \quad (C4)$$

**APPENDIX D: QUANTUM FLUCTUATIONS IN CURRENT**

Quantum noise is defined as

$$\overline{N} = \frac{1}{2} \langle\{\hat{I}(t) - \hat{I}(0)\}, \hat{I}(t) - \hat{I}(0)\rangle \quad (D1)$$

or, equivalently,

$$\overline{N} = \frac{1}{2} \langle\{\hat{I}(t), \hat{I}(0)\}\rangle - \hat{I}(0)\hat{I}(t). \quad (D2)$$

We recall that the current operator can be written as

$$\hat{I}(t) = -\frac{e\hbar}{2} \left[\sum_{j \in L,R} \tilde{\iota}_j (d_j^\dagger(t)c_j(t) - c_j^\dagger(t)d_j(t))\right],$$

where

$$\tilde{\iota}_j = \iota_j \quad \text{if} \quad j \in L$$

$$= -\iota_j \quad \text{if} \quad j \in R. \quad (D3)$$

Therefore, the quantum noise operator is given by:

$$\hat{N} = -\frac{e^2}{8\hbar^2} \sum_{i,j} \tilde{\iota}_i \tilde{\iota}_j [d_i^\dagger(t)c_i(t)d_i(t)c_i^\dagger(t) - c_i^\dagger(t)c_i(t)d_i^\dagger(t)c_i(t) - d_i^\dagger(t)c_i(t)c_i^\dagger(t)d_i(t) + c_i(t)c_i^\dagger(t)d_i^\dagger(t)c_i(t) - d_i(t)c_i^\dagger(t)c_i(t)d_i^\dagger(t)c_i(t) - c_i^\dagger(t)d_i(t)d_i^\dagger(t)c_i(t) + c_i^\dagger(t)d_i(t)c_i^\dagger(t)d_i(t)] - \hat{I}(t)\hat{I}(t). \quad (D4)$$
The time dependence of the operators $c_i(t)$ can all be written down in terms of the eigenvalues $\epsilon_a$ and wave functions $\psi_a(t)$ of the hopping matrix $T_{ij}$. Assuming that the wave functions $\psi_a(t)$ of the hopping matrix are all real (they can be made to be real since the hopping matrix is real and symmetric), we can, after a long, tedious calculation, write down a compact expression for quantum noise:

$$\overline{N} = -\frac{e^2}{4\hbar^2} \sum_{k,l} \text{Re} \left[ U_{kl}(t) V_{kl}(t_0) \right] - I(t) I(t_0),$$

where the complex matrices $U, V$ are defined as follows:

$$U_{kl}(t) = W_{nk}(t) \sum_j \tilde{t}_j W_{jk}^*(t),$$

$$V_{kl}(t_0) = (f_k + f_l - 2 f_k f_l) \left[ W_{Nl}(t_0) \sum_j \tilde{t}_j W_{jk}^*(t_0) - W_{Nk}(t_0) \sum_j \tilde{t}_j W_{jl}(t_0) \right] + i 4 \delta_{kl} f_l \text{Im} \left[ \sum_{jm} \tilde{t}_j f_m W_{Nm}(t_0) W_{jm}^*(t_0) \right],$$

where the matrix $W(t)$ is defined as

$$W_{mn}(t) = \sum_a e^{i \epsilon_a t} \psi_a(m) \psi_a(n),$$

and $f_k, k = 1, \ldots, (N-1)$ are the Fermi-Dirac distribution functions for the left and right leads and $f_N = n_0$ is the initial dot population, which together define the initial density matrix of our system. In the above equations, the indices $k,l,m,n$ can all take values from $1,\ldots,N$, i.e., the left and right leads and the dot, the label $N$ referring to the quantum dot. When we consider the above quantum noise at a particular instance of time, it is just the quantum fluctuation in current,

$$\overline{N} = \langle \hat{J}(t)^2 \rangle - I(t)^2,$$

which can again be computed by the methods described above.