Many-body current formula and current conservation for non-equilibrium fully interacting nanojunctions

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1. Introduction

Electronic transport through molecular nanojunctions exhibits many important new features in comparison with conduction through macroscopic systems such as bulk or thin layers of semi-conducting molecular crystals as used in conventional molecular electronics. In particular, local interactions, such as Coulomb interactions between the electrons and scattering from localized
atomic vibrations, become critically important. In crude terms, these interactions are more pronounced in nanoscale systems because the electronic probability density is concentrated in a small region of space; normal screening mechanisms are thus ineffective. Developing a theory for the non-equilibrium electronic quantum transport through such fully interacting nanoscale junctions is a challenging task, especially when thinking in terms of applications for future nanoscale electronics.

Having a simple expression for the electronic current or for the conductance of a nanoscale object connected to terminals is most useful. This is provided by the Landauer formula [1] in the form of an appealing intuitive physical picture, which describes the current in terms of local properties of a finite region (transmission coefficients) and the statistical distribution functions of the electron reservoirs connected to the central region $C$. However, in its original form the Landauer formula deals only with non-interacting electrons. This formalism has been used in conjunction with density-functional theory (DFT) calculations for realistic nanoscale systems [2–12]. It has helped tremendously for the qualitative understanding of the transport properties of such realistic systems, though only on a semi-quantitative level as the calculated conductance is often one or two orders of magnitude wrong. The apparent success of such an approach relies on the fact that DFT maps the many-electron interacting system onto an effective non-interacting single-particle Kohn–Sham Hamiltonian suited for the Landauer scattering formalism for transport. However, there are many cases when such a mapping becomes questionable: for strongly interacting electron systems, low-dimensional interacting electron system, strongly coupled electron–phonon systems, to cite only a few.

Furthermore, the single-particle framework of the Landauer approach cannot be directly transferred to the many-body context by expecting that a proper inclusion of many-body effects in the single-particle energy levels will suffice. In fact, it has been shown that there are many-body corrections to the Landauer formula which cannot be formulated in terms of single-particle transmission probabilities [13, 14].

When a single-particle-like scheme is still valid even in the presence of interaction, the Landauer approach can be extended to include inelastic effects by using inelastic scattering theory in a generalized Fock-like space [15–22].

In the context of DFT, it has also been shown that the exchange-correlation part of the interaction that leads to the presence of an extra $v_{xc}$ potential is actually introducing corrections to the Landauer-like current. These corrections are crucial and need to be taken into account when working with DFT calculations [23, 24]. The Landauer formula has been built upon by Meir and Wingreen [25] to extend this formalism to a central scattering region $C$ containing interactions between particles, while the left ($L$) and right ($R$) leads are still represented by non-interacting electron seas. The current is then expressed in terms of non-equilibrium Green’s functions (NEGF) and self-energies, and in the most general cases it does not bear any formal resemblance to the original Landauer formula for the current [26, 25, 27]. Other generalizations of Landauer-like approaches to include interactions and inelastic scattering have been developed; see, for example, [22, 28, 29, 13]. The Meir and Wingreen partition scheme has also been extended to deal with nonorthogonal basis sets [30].

However, in real systems the interaction is present throughout the entire system, even at the nanoscale. This is even more true for the long-range Coulomb interaction between bare electrons. Hence, it is difficult to consider that in the real system all kinds of interactions will stay localized or will be sufficiently well described by the localized effective interaction in the $C$ region only. Another reason is that in time-dependent transport, the external field in the leads may not necessarily be screened instantaneously. Transient times can be of the same order as the plasma oscillation (a collective many-body mode of charge oscillation) period in leads and
play an important role in the transient transport properties of the nanojunction [31]. Taking the interaction into the whole system is vital. To achieve this, the so-called partition-free scheme has been developed [32]. It allows in principle the calculation of physical dynamical responses and to include the interactions between the leads and between the leads and the central region in a quite natural way [33, 34].

In this paper, we use an alternative approach and generalize the Meir and Wingreen formalism (so-called partitioned scheme) to systems where interaction exists in all the $L, C, R$, as well as at the interfaces between the three regions. Since the choice of location of these interfaces is purely arbitrary and since the interactions exist at and on both sides of the interface, our approach is equivalent to a partition-free scheme.

However, while keeping the approach and the NEGF formalism of the original work of Meir and Wingreen [25], we derive the most general expression of the current for the fully interacting system. From this, we can recover all previously derived transport expressions or corrections when introducing the appropriate level of approximation for the interaction. We also derive and study in detail the current conservation condition and the constraint that it imposes on the interaction self-energies.

Our formalism also introduces naturally the generalization of the concept of the embedding potential when the interaction crosses at the boundaries. With this new concept and with the condition of current conservation, we can explore different levels of approximation for treating the interaction in the different parts of the system, as well as at the interface. We can then check which approximations are more suitable for practical numerical calculations of realistic systems.

Although a preliminary account of our formalism is already given in [35], we provide here the full details of the derivation and a much more detailed discussion of the physical meaning of our results as well as of the implementation of the present formalism for realistic calculations.

The paper is organized as follows. We start with the description of the system and the notation in section 2. Then, we derive the expression for the current for the fully interacting system in section 3. We provide the full derivation of the expressions for the different Green functions needed to calculate the current in section 4. We derive the conditions imposed by the constraint of current conservation in section 5. We finally conclude and discuss open questions as well as different schemes to perform the calculation for realistic systems in section 6. We recall some properties of the Green functions and self-energies in appendices A and B, and provide the proof of an important relation for the current conservation in appendix C.

2. System model

The system consists of two electrodes, labelled $L$ and $R$ for left and right, respectively, which connect a central region $C$ via a set of coupling matrix elements $V_{LC,RC}$. The interaction—which we specifically leave undefined (e.g. electron–electron or electron–phonon)—is assumed to be well described in terms of the single-particle self-energy $\Sigma_{MB}$ and spreads over the entire system.

For the calculation of the current, we introduce two interfaces $LC$ and $RC$ defining the three regions $L, C$ and $R$ and use different labels to name the electronic states on each side of these interfaces. The labels $\{\lambda, \lambda', \{n, m\}, \{\rho, \rho'\}$ are used to represent the complete and orthogonal set of states for the $L, C$ and $R$ regions, respectively.

In the following, we will use either the full notation or a compact notation for the Green functions $G$ and the self-energy $\Sigma$. Following figure 1, the matrix elements of $M_{ij}$ of a Green function or of a self-energy are annotated $M_{ij}$ for the matrix elements of the central region.
Figure 1. Schematic representation of a central scattering region C connected to the left L and right R electrodes, with respective quantum-state labels $\{\lambda\}, \{n\}, \{\rho\}$ for the three L, C, R subspaces. The electronic coupling of the region C to the L(R) region is given by $V_{LC}/V_{CL}$, and the many-body interaction is represented by $\Sigma_{mb}$ within all regions as well as across the LC and CR interfaces. The LC/R interfaces can be chosen to be located at the contacts between the molecule and the leads, or inside the leads (as shown above).

$M_{mn}$. We use the notation $M_L$ for $M_{\lambda\lambda'}$ and $M_R$ for $M_{\rho\rho'}$. The matrix elements are also annotated $M_{LC}$ for $M_{\lambda m}$ or $M_{CL}$ for $M_{\lambda'}m$, and $M_{RC}$ for $M_{\rho m}$ or $M_{CR}$ for $M_{\rho'}m$. For the hopping matrix elements, we use $V_{\lambda m}$ or $V_{\rho m}$ for $V_{LC}$ or $V_{CL}$ at the left interface and $V_{\lambda'}m$ or $V_{\rho'}m$ for $V_{RC}$ or $V_{CR}$ at the right interface.

3. The current formula

3.1. NEGFs on the Keldysh contour $C_K$

The Green function on the Keldysh contour $C_K$ is defined as

$$G(1, 2) = -i \langle T_{C_K} \Psi(1) \Psi^\dagger(2) \rangle,$$

where $(1, 2)$ stands for a composite index for space $x_1, x_2$ (i.e. states $\lambda, n$ or $\rho$ in the L, C or R regions, respectively) and time $\tau_1, \tau_2$ on the time-loop contour $C_K$. The time ordering $T_{C_K}$ of the product of fermion creation ($\Psi^\dagger$) and annihilation ($\Psi$) quantum fields is performed on the time-loop contour $C_K$ [36–39].

The Green function obeys the equation of motion on the contour $C_K$ [37, 39]:

$$[i \partial_{\tau_1} - \tilde{h}_0(1)]G(1, 1') = \delta(1 - 1') + \int d3 \Sigma(1, 3) G(3, 1'),$$

and the adjoint equation reads

$$[-i \partial_{\tau_1'} - \tilde{h}_0(1')]G(1, 1') = \delta(1 - 1') + \int d2 G(1, 2) \Sigma(2, 1'),$$

where $\tilde{h}_0(1)$ is the non-interacting Hamiltonian.

3.2. The current

Using the continuity equation $\nabla \cdot j(1) + \partial_t n(1) = 0$, one can write down the current through the interface between the L and C regions. It should be noted that considering an interface between the L (R) and C regions is merely a virtual partitioning for mathematical convenience—the interactions are present throughout the entire system. It is also useful to consider such L/C interfaces in order to connect our results to previously derived expressions within the partitioning scheme. The location of these interfaces is also arbitrary, but for convenience in future numerical computation, different choices are possible: for example, at the contacts between the leads and the ends of the molecule, or at the contacts between the leads and the so-called extended molecule, which already contains part of the leads.
After integration of the continuity equation over the (half) space of the $L$ region, one obtains the following expression for the current flowing through the left interface (from $L$ to $C$):

$$I_L(t) = -\frac{e}{\hbar} \frac{d}{dt} \langle \hat{N}_L(t) \rangle,$$

where $\langle \hat{N}_L(t) \rangle$ is the total number of electrons in the $L$ region. It is obtained from the lesser Green function as

$$\langle \hat{N}_L(t) \rangle = \sum_\lambda -iG^<_{\lambda\lambda}(t,t).$$

To calculate the time derivative of $G^<_{\lambda\lambda}(t,t)$, we first go back to the full two-time dependence of $G^<$, and then take the equal-time limit after performing the derivatives:

$$\frac{d}{dt} \langle \hat{N}_L(t) \rangle = \sum_\lambda \left( -i \frac{d}{dt_1} G^<_{\lambda\lambda}(t_1,t) - i \frac{d}{dt_2} G^<_{\lambda\lambda}(t,t_2) \right) \bigg|_{t_1=t_2=t}.$$  

Using the equations of motion, equations (2) and (3), for the Green functions on $C$, one obtains the current $I_L$ as

$$I_L(t) = \frac{e}{\hbar} \text{Tr}_L[(\Sigma G)^<(t,t) − (G\Sigma)^<(t,t)],$$

where we have re-introduced the $\hbar$ to have the correct units of current and conductance.

Using the rules of analytical continuation (see appendix B), we get

$$\text{Tr}_L[\ldots] = \text{Tr}_L[(\Sigma^{MB})^<(t,t) + (V_{LC} + \Sigma^{MB,r})(t,t)G^<]$$

$$− (G^<(V_{LC} + \Sigma^{MB,a})(t,t) − (GΣ)^<(t,t)].$$

There are no lesser and greater components for $V_{LC}$ since its time dependence is local, i.e. $V_{LC}(t,t') = V_{LC}(t)\delta(t-t')$.

In the steady state, all double-time quantities $X(t,t')$ depend only on the time difference $X(t-t')$. One obtains the following expression for the current $I_L$ after the Fourier transform

$$I_L = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}_L[(\Sigma(\omega)G(\omega))^<(t,t) − (G(\omega)\Sigma(\omega))^<]$$

or equivalently

$$I_L = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}_L[V_{LC}G^<(\omega) − G^<(\omega)V_{LC} + \Sigma^{MB,a}(\omega)G^<(\omega) + \Sigma^{MB,r}(\omega)G^<(\omega) − G^<(\omega)Σ^{MB,a}(\omega) − G^<(\omega)Σ^{MB,r}(\omega)].$$

Now that we have sorted out the Keldysh components, we have to sort out the index (matrix elements) parts. First we concentrate on $\text{Tr}_L[(\Sigma^{MB}G)^<$] and $\text{Tr}_L[(G\Sigma^{MB})^<$]. We thus have (we use the symbol $\sum$ for summation to have a better graphical distinction between the sums and the self-energies $\Sigma$):

$$\text{Tr}_L[(\Sigma^{MB}G)^<] = \sum_{\lambda,\alpha} (\Sigma_{\lambda\alpha} G_{\alpha\alpha})^< + \sum_{\lambda,\lambda'} (\Sigma_{\lambda\lambda'} G_{\lambda\lambda'})^< + \sum_{\lambda,\rho} (\Sigma_{\lambda\rho} G_{\rho\rho})^<.$$  

and similarly for $\text{Tr}_L[(G\Sigma^{MB})^<$]:

$$\text{Tr}_L[(G\Sigma^{MB})^<] = \sum_{\lambda,\alpha} (G_{\lambda\alpha} \Sigma_{\alpha\alpha})^< + \sum_{\lambda,\lambda'} (G_{\lambda\lambda'} \Sigma_{\lambda\lambda'})^< + \sum_{\lambda,\rho} (G_{\lambda\rho} \Sigma_{\rho\rho})^<.$$  

In this present version of the theory, we assume that the matrix elements $\Sigma_{\rho\rho}$ and $\Sigma_{\lambda\rho}$ vanish, as there is no direct interaction between the left and right electrode. Because of the geometry
and the heterogeneity of the nanojunctions and because of the different dimensionality of the leads and the central region, we assume that there is an effective screening of the Coulomb interaction so that the electrons of the $L$ and $R$ leads do not interact directly via any $\Sigma_{\lambda\rho}^{\text{MB}}$ or $\Sigma_{\lambda\rho}$ matrix elements. The distance $|\mathbf{x}_i - \mathbf{x}_j|$ between two points in the $L$ and $R$ leads respectively is large enough so that the spatial decay of $\Sigma_{\lambda\rho}^{\text{MB}}(\mathbf{x}_i - \mathbf{x}_j)$) make the contribution of $\Sigma_{\lambda\rho}^{\text{MB}}$ zero or negligible. In other words, the presence of the $L$ and $R$ electrodes affect directly the central region $C$ via $\Sigma_{\lambda\rho}^{\text{MB}}$ and $\Sigma_{\lambda\rho}^{\text{RC}}$. However, the $L$ electrode do not affect directly the $R$ electrode (and vice versa), but only indirectly via exchange and correlation effects involving the states of the central region $C$. This assumption seems to be valid when the size of the central region is of the order of several atoms (i.e. a molecule). If the central region were to be a single atomic impurity coupled to two continuum of the delocalized electron state, this assumption would not be valid.

We now turn to the evaluation of the sums in equations (11) and (12). First we concentrate on the $\Sigma_{\lambda,\lambda}'$ sums

$$
\sum_{\lambda,\lambda'} (\Sigma_{\lambda,\lambda}^{\text{MB}} G_{\lambda,\lambda'}) < - \sum_{\lambda,\lambda'} (G_{\lambda,\lambda'} \Sigma_{\lambda,\lambda}^{\text{MB}}) <
$$

$$
= \sum_{\lambda,\lambda'} \Sigma_{\lambda,\lambda}^{\text{MB},<} G_{\lambda,\lambda'}^{<} + \Sigma_{\lambda,\lambda'}^{\text{MB},>} G_{\lambda,\lambda'}^{<} - G_{\lambda,\lambda'}^{<} \Sigma_{\lambda,\lambda}^{\text{MB},<} - G_{\lambda,\lambda'}^{<} \Sigma_{\lambda,\lambda}^{\text{MB},>}
$$

$$
= \sum_{\lambda,\lambda'} \Sigma_{\lambda,\lambda}^{\text{MB},<} (G_{\lambda,\lambda'}^{<} - G_{\lambda,\lambda'}^{<}) + (\Sigma_{\lambda,\lambda}^{\text{MB},<} - \Sigma_{\lambda,\lambda}^{\text{MB},>}) G_{\lambda,\lambda'}^{<}
$$

$$
= \sum_{\lambda,\lambda'} \Sigma_{\lambda,\lambda}^{\text{MB},<} G_{\lambda,\lambda'}^{<} - \Sigma_{\lambda,\lambda}^{\text{MB},<} G_{\lambda,\lambda'}^{<} = \text{Tr}_x \left[ \Sigma_{\lambda}^{\text{MB},>} G_{\lambda}^{<} - \Sigma_{\lambda}^{\text{MB},<} G_{\lambda}^{<} \right].
$$

In the second line, we have used the rules of analytical continuation. In the third, we have used the equivalent of cyclic permutation in the calculation of a trace, i.e. swapping the indices $\lambda$ and $\lambda'$ in the last two terms. This is possible here since the sums and all matrix elements are defined in the single subspace of the $L$ electrode. The final result looks like the collision terms usually obtained in the derivation of the generalized Boltzmann equation from quantum kinetic theory. They correspond to the particle production (scattering-in) and absorption or hole production (scattering-out) related to inelastic processes (i.e. non-diagonal elements of the self-energy on the time-loop contour $\Sigma$) occurring in the left electrode. It has also been shown that the integration of such term vanishes as a result of the gauge degree of freedom [40]. In section 3.4, we use another route to show how and why these terms can vanish by using generalized non-equilibrium distribution functions.

Now let us concentrate on the $\Sigma_{\lambda,\lambda}'$ sums in equation (11) and equation (12). Once more using the rules of analytical continuation, we can see that we need the knowledge of the following Green’s functions matrix elements: $G_{\lambda\lambda}^{<}$, $G_{\lambda\alpha}^{<}$, $G_{\alpha\lambda}^{<}$ and $G_{\alpha\alpha}^{<}$. For this we use the Dyson-like equation defined for the non-diagonal elements: $G_{\lambda\lambda}^{<} = \langle n | (G \Sigma g)^{<} | \lambda \rangle$. We will not go into the detail of the full calculations for all four Green’s function matrix elements; instead we concentrate on one matrix element $\langle n | (G \Sigma g)^{<} | \lambda \rangle$ to show the mechanism of the derivation

$$
G_{\lambda\lambda}^{<} = \langle n | (G \Sigma g)^{<} | \lambda \rangle = \langle n | G^{<} \Sigma^{<} g^{>} + G^{>} \Sigma^{>} g^{<} + G^{<} \Sigma^{>} g^{>} | \lambda \rangle
$$

$$
= \sum_{\lambda_{1}, \lambda_{2}, \rho, \mu, m} G_{\lambda_{1}\lambda_2}^{<} \Sigma_{\lambda_{1}\lambda_2}^{<} g_{\lambda_{1}\lambda_2}^{>} + G_{\lambda_{2}\lambda_1}^{<} \Sigma_{\lambda_{2}\lambda_1}^{<} g_{\lambda_{2}\lambda_1}^{>} + G_{\mu m}^{<} \Sigma_{\mu m}^{<} g_{\mu m}^{>}
$$

$$
= \sum_{\lambda_{1}, \lambda_{2}, \rho, \mu, m} G_{\lambda_{1}\lambda_2}^{<} \Sigma_{\lambda_{1}\lambda_2}^{<} g_{\lambda_{1}\lambda_2}^{>} + G_{\lambda_{2}\lambda_1}^{<} \Sigma_{\lambda_{2}\lambda_1}^{<} g_{\lambda_{2}\lambda_1}^{>} + G_{\mu m}^{<} \Sigma_{\mu m}^{<} g_{\mu m}^{>}
$$

6
Eqs. (17), (18) and (19) are the main results of this work for the current formula. The where

\[\Sigma_{\mu L} = V_{\mu L} + \Sigma_{\mu L}^{MB, a/r} \text{ and } \Sigma_{\mu L}^{<} = \Sigma_{\mu L}^{MB, <}.\]

One has to keep in mind that we use a model such that \(\Sigma_{\mu L}^{<} = 0\).

As we show in detail in section 4.1, the interaction defined within the subspace of the L lead \(\Sigma_{\mu L}^{a/r}\) can be factorized out and included in the renormalized Green functions \(\tilde{g}_{\lambda L}^{r}\) of the L lead. Hence, the matrix elements \(G_{\lambda}^{<} = \langle n|G_{\lambda}^{<}|n\rangle\) can be recast as

\[G_{\lambda}^{<} = \sum_{m, n} G_{nm}^{m} \Sigma_{\mu L}^{<} \tilde{g}_{\lambda L}^{<} + G_{nm}^{<} \Sigma_{\mu L}^{MB, <} \tilde{g}_{\lambda L}^{<} + G_{nm}^{<} \Sigma_{\mu L}^{MB, <} \tilde{g}_{\lambda L}^{<}.\]  

Similarly, we find that

\begin{align*}
G_{\lambda}^{a} &= \langle \lambda | (g_{LC} G_{C})^{a} | n \rangle, \\
G_{\lambda}^{m} &= \langle n | (G_{C} \Sigma_{\mu L}^{a} g_{LC}^{m})^{a} | \lambda \rangle, \\
G_{\lambda}^{r} &= \langle \lambda | (\tilde{g}_{LC} G_{C})^{r} | n \rangle.
\end{align*}

Finally by using the rules of analytical continuation for the above matrix elements, we find that the current flowing through the left L interface (10) can be recast as

\[I_{L} = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}_{a}[G_{C}^{<} \tilde{\gamma}_{C}^{L} + G_{C}^{<} (\tilde{\gamma}_{C}^{L})^{+} + G_{C}^{<} (\tilde{\gamma}_{C}^{L} - (\tilde{\gamma}_{C}^{L})^{+})] + \text{Tr}_{a} \left[\Sigma_{L}^{MB, <} G_{C}^{<} - \Sigma_{L}^{MB, <} G_{C}^{<}\right].\]  

(17)

where

\[\tilde{\gamma}_{C}^{L} = \Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c},\]

\[\tilde{\gamma}_{C}^{L} = \Sigma_{\mu L}^{a} (\tilde{g}_{L}^{a} - \tilde{g}_{L}^{a}) \Sigma_{\mu L}^{c} + \Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c}\]

\[= (\Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c} - \Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c})^{+}.\]  

(18)

and

\[\left(\tilde{\gamma}_{C}^{L}\right)^{+} = \Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c},\]

\[\left(\tilde{\gamma}_{C}^{L}\right)^{+} = \Sigma_{\mu L}^{a} (\tilde{g}_{L}^{a} - \tilde{g}_{L}^{a}) \Sigma_{\mu L}^{c} - \Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c}\]

\[= (\Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c} - \Sigma_{\mu L}^{a} \tilde{g}_{L}^{a} \Sigma_{\mu L}^{c})^{+}.\]  

(19)

Equations (17), (18) and (19) are the main results of this work for the current formula. The current \(I_{L}\) flowing at the left LC interface is given by two traces: the first trace is a generalization of the Meir and Wingreen expression of the current to the cases where there are both interactions within the left electrode and crossing at the LC contact. The second trace is a term related to inelastic transport effects involving summation over the left electrode states/sites only.

An expression similar to equation (17) can be obtained for the current \(I_{R}\) flowing at the right RC interface, by swapping the index \(L \leftrightarrow R\) and changing the sign to keep the same convention for positive current flowing from the left to right direction. We find

\[I_{R} = -\frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}_{a}[G_{C}^{<} \tilde{\gamma}_{C}^{R} + G_{C}^{<} (\tilde{\gamma}_{C}^{R})^{+} + G_{C}^{<} (\tilde{\gamma}_{C}^{R} - (\tilde{\gamma}_{C}^{R})^{+})] + \text{Tr}_{a} \left[\Sigma_{R}^{MB, >} G_{R}^{<} - \Sigma_{R}^{MB, <} G_{R}^{<}\right].\]  

(20)

We now comment on the physical meaning and implication of the new \(\gamma_{C}^{a}\) quantities and the different traces entering the definition of the current.
3.3. Relationships between the $\tilde{\chi}_L^C$ quantities

From the definition of $\tilde{\chi}_L^C$, equation (18), we can also define the quantity $\tilde{\chi}_L^{C L}$ using the greater components $\Sigma_{CL}^>$ and $\tilde{g}_L^>$ such as

$$\tilde{\chi}_L^{C L} = \Sigma_{CL}^> (\tilde{g}_L^> - \tilde{g}_L^<) \Sigma_{CL}^r + \Sigma_{CL}^L \tilde{g}_L^< \Sigma_{LC}^r.$$

(21)

It is now easy to show that $\tilde{\chi}_L^C$ and $\tilde{\chi}_L^{C L}$ are related to each other by

$$\tilde{\chi}_L^{C L} - \tilde{\chi}_L^C = \{\tilde{\chi}_L^C\} - \tilde{\chi}_L^C.$$

(22)

This is a very interesting relationship in the sense that the $\tilde{\chi}_L^C$ quantities obey a relation of the type (greater) − (lesser) = (retarded) − (advanced) as for conventional self-energies or Green’s functions, though $\tilde{\chi}_L^{C L}$ and $\tilde{\chi}_L^C$ are not proper lesser and greater quantities. It should also be noted that the different $\tilde{\chi}_L^{C L}(\omega)$ play a similar role as the lead self-energies (or embedding potentials [41–43]), defined as $\Sigma_{CL}^{\text{MB}}(\omega) = V_{CL} g_{L}^{>}(\omega) V_{LC}$ when the interactions are not crossing at the contacts. However, they are not simply related to the straightforward generalization of these embedding potentials. The latter have the following form (see also the expression for the Green functions given in section 4)

$$\tilde{\chi}_L^{C L}(\omega) = (\Sigma_{CL}^L(\omega) \tilde{g}_L^<(\omega) \Sigma_{LC}^r(\omega))^x,$$

(23)

with $\Sigma_{LC/C}(\omega) = V_{CL}/CL + \Sigma_{MC/C}(\omega)$ and $x = (>,<,r,a)$. The rules of analytical continuation for $\tilde{\chi}_L^{C L}$ and $\tilde{\chi}_L^{C r}$ do not give the same expression as for $\tilde{\chi}_L^C$ or $\tilde{\chi}_L^{C L}$. For example, $\tilde{\chi}_L^{C L} = \Sigma_{CL}^> g_L^> \Sigma_{LC}^r \neq \tilde{\chi}_L^C$ and $\tilde{\chi}_L^{C r} \neq \tilde{\chi}_L^C$.

This leads us to an important proof of this work: because of (a) the very existence of the interaction crossing at the contact, of (b) the fact that $\Sigma_{La/ac}^a \neq \Sigma_{La/ac}^r$ as opposed to the non-interacting case where $V_{La/ac} = V_{La/ac} = V_{La/ac}$, and of (c) the rules of analytical continuation for products of three quantities, the usual cyclic permutation used in the calculation of the trace $\text{Tr}_\lambda[(\Sigma G)^{-} - (G \Sigma)^{-}]$ cannot be used to transform the initial trace over $\lambda$ onto a trace over $\alpha$. Therefore, the current $I_L$ at the LC contact cannot be expressed simply in terms of the generalized embedding potentials $\tilde{\chi}_L^{C,L}$; hence, the introduction of the $\tilde{\chi}_L^C$ quantities. The current is not obtained from a straightforward generalization of the Meir and Wingreen formula using the embedding potentials $\tilde{\chi}_L^{C,L}$:

$$I_L \neq e \int \frac{d\omega}{2\pi} \text{Tr}_\lambda \left[ Y_L^{\lambda-} G_C^\lambda - Y_L^{\lambda+} G_C^\lambda \right] + \text{Tr}_\lambda \left[ \Sigma_{L}^{\text{MB},-} G_C^\lambda - \Sigma_{L}^{\text{MB},+} G_C^\lambda \right].$$

(24)

3.4. Non-equilibrium distribution functions in the leads

Now we consider the terms $\text{Tr}_\lambda \left[ \Sigma_{L}^{\text{MB},-} G_C^\lambda - \Sigma_{L}^{\text{MB},+} G_C^\lambda \right]$ and show in which conditions this trace vanishes. For this we introduce the non-equilibrium distribution functions $f_L^{\lambda-}(\omega)$ and $f_L^{\lambda+}(\omega)$ defined from the generalized Kadanoff–Baym ansatz [44] as follows:

$$G_C^\lambda(\omega) = f_L^{\lambda-}(\omega) G_C^L(\omega) - G_L^\lambda(\omega) f_L^{\lambda+}(\omega),$$

$$\Sigma_L^{\text{MB},-}(\omega) = f_L^{\text{int},-}(\omega) \Sigma_L^{\text{MB},a}(\omega) - \Sigma_L^{\text{MB},+}(\omega) f_L^{\text{int},-}(\omega).$$

(25)

and similarly for $f_L^{\lambda+}$ and $f_L^{\text{MB},+}$, obtained from $G_C^\lambda$ and $\Sigma_{L}^{\text{MB},+}$. These distribution functions follow the conditions $f_L^{\lambda-} = f_L^{\lambda-} - 1_L$ and $f_L^{\text{int},-} = f_L^{\text{int},-} - 1_L$ (where the identity matrix in the $L$ region is $1_L = \delta_{\lambda,\lambda'}$ so that the usual relationships between the different Green functions (and self-energies) $X' - X = X - X'$ still hold.

For convenience, we consider for the moment that the non-equilibrium distribution functions are diagonal in the corresponding subspace, i.e. $f_{\lambda,\lambda'}^{\lambda,\lambda'} = f_{\lambda,\lambda'}^{\lambda,\lambda'} \delta_{\lambda,\lambda'}$. However, there is
no formal difficulty to deal with a full, non-diagonal, dependence of these density-matrix-like distribution functions.

Introducing the definition of the non-equilibrium distribution functions in equation (13), we end up, after lengthy (but rather trivial) calculations, with

\[
\text{Tr} \left[ \Sigma_{MB} - G_\lambda \right] = (2\pi)^2 \text{Tr} \left[ \frac{f_\lambda - f_{\text{int}}^\text{eq}}{\Sigma_1 L} A_L^\lambda A_L^\lambda \right],
\]

(26)

where the respective spectral functions are obtained from

\[
2\pi i A_L^\lambda (\omega) = X(a)_L (\omega) - X(r)_L (\omega),
\]

(27)

Equation (26) shows that the collision term is a measure of the deviation between the two distribution functions \( f_\lambda \) and \( f_{\text{int}}^\text{eq} \). At equilibrium, because all distribution functions are equal to the Fermi distribution \( f_\lambda = f_{\text{int}}^\text{eq} \), this collision term vanishes. At non-equilibrium this is not generally the case.

One can now imagine the following case: the indices \( \lambda \) represent a spatial location or a localized electronic state on a lattice point in the left electrode. For \( \lambda \) located well inside the electrode, the system is in its local equilibrium (the Fermi distribution with a Fermi level shifted by the left bias) and both distribution functions \( f_\lambda \) and \( f_{\text{int}}^\text{eq} \) are equal to the left Fermi distribution; hence, these indices do not contribute to the trace. Only the lattice points (or states) that are not in local quasi-equilibrium, i.e. those close enough to the central region to experience the potential drop and the interaction effects at the contact and beyond will contribute to the trace. From a computational point of view, this is good news in the sense that one is not obliged to perform the summation in \( \text{Tr} [...] \) over all the infinite \( \lambda \) indices of the semi-infinite left electrode. Only the states/sites for which \( f_\lambda - f_{\text{int}}^\text{eq} \neq 0 \) will contribute to the trace. So if we choose the location of the LC interface far enough inside the left electrode of the real system, then \( \text{Tr} [...] = 0 \). In this sense, we have just provided a formal proof of the concept of the so-called extended molecule [45, 10, 9, 6, 46, 47]. The extended molecule not only represents the central region \( C \) and consists of the molecule itself but also a part of the left and right electrodes to which the molecule is connected. The concept of the extended molecule has been introduced empirically in realistic calculations of molecular junctions in order to avoid any problems with the asymptotic behaviour of the electrostatic potential in the bias of finite (not small) applied bias.

The value of \( \text{Tr} [...] \) can also be understood as a measure of the ‘efficiency’ of the location of the LC interface in the L electrode. The larger (smaller) the value is, the farther (closer) from local equilibrium the LC interface is. This measure can help in finding a good compromise between having a sufficiently large extended molecule that is nonetheless small enough for tractable numerical calculations.

3.5. The Meir and Wingreen current formula

Using different approximations (for example, single-particle approaches, mean-field theories, interactions localized in the central region only) for the different interacting self-energies, we can recover from equation (17) all the previously derived current expressions for non-equilibrium nanojunctions. We have analysed all these connections in detail in [35] and we will not repeat the analysis here.

However, as will be useful below, we now briefly recall that equation (17) bears some resemblance to the current expression derived by Meir and Wingreen [25] in the case of interaction present in the central region only:

\[
I_{\text{MW}}^L = \frac{i e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}_n \left[ f_L (G_C^\text{eq} - G_C^\text{eq}) \Gamma_C^L + G_C^\text{eq} \Gamma_C^L \right].
\]

(28)
The connection becomes more apparent when we use the definitions \( i_{CL} = V_{CL} \) and \( i_{RL} = V_{RL} \). Hence, \( I_{L}^{\text{MW}} \) becomes
\[
I_{L}^{\text{MW}} = e \int \frac{\text{d} \omega}{2\pi} \text{Tr}_{\alpha} \left[ G_{C}^{-} \Sigma_{L}^{-} + G_{C}^{-} \left( \Sigma_{C}^{-} + \Sigma_{C}^{L^{-}} \right)^{-1} G_{C}^{-} \right].
\] (29)

One can see by comparing equations (17) and (29) that the quantities \( \tilde{\Sigma}_{C}^{L^{-}} \), \( \left( \tilde{\Sigma}_{C}^{L^{-}} \right)^{-1} \) and \( \tilde{\Sigma}_{C}^{L^{-}} \) play the role of the L lead self-energies \( \Sigma_{C}^{L^{-}}, \Sigma_{C}^{L^{-}} \) and \( \Sigma_{C}^{L^{-}} \), respectively, in the cases where the interactions cross at the L interface. However, as we have discussed above, the quantities \( \tilde{\Sigma}_{C}^{L^{-}} \) are the forward generalization of the embedding potentials \( \tilde{\Sigma}_{C}^{L^{-}} \). Note that, in the model of Meir and Wingreen, the leads are non-interacting; hence, the second trace \( \text{Tr}_{\alpha} \ldots \) in equation (17) vanishes.

4. The different Green functions needed

For the evaluation of the currents \( I_{L} \) and \( I_{R} \), we need to know the following Green functions \( G_{C}^{\alpha/\gamma} \) and \( G_{C}^{\alpha/\gamma} \). Here we calculate the matrix elements: \( G_{C}^{\alpha} = \langle n | (g + g \Sigma G)^{\alpha} | n \rangle \), \( G_{C}^{\gamma} = \langle \rho | (g + g \Sigma G)^{\gamma} | \rho \rangle \). The results are given in the following subsections.

4.1. Renormalization of the Green functions in the electrodes

First we show that the terms in \( \Sigma_{L}^{L^{-}} \) can be factorized out and included within the renormalization of the left lead Green functions \( G_{L}^{\alpha/\gamma} \). Hence, the matrix elements \( G_{L}^{\alpha} = \langle n | (G \Sigma G)^{\alpha} | \lambda \rangle \) can be recast as \( G_{L}^{\alpha} = \langle n | G_{C}^{-} \Sigma_{C}^{-} \tilde{G}_{L} G_{C}^{-} | \lambda \rangle \) with \( \tilde{G}_{L} \) the renormalized L lead Green function whose definition is given below.

We start from
\[
G_{m}^{\alpha} = \langle n | (G \Sigma g)^{-1} | \lambda \rangle
= \sum_{\xi, \xi', n} G_{m}^{\alpha} \Sigma_{\xi, \xi'}^{\alpha} g_{\xi, \xi'} + G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi} + G_{m}^{\gamma} \Sigma_{\xi, \xi'}^{\gamma} g_{\xi, \xi'} + G_{n}^{\gamma} \Sigma_{n, \xi}^{\gamma} g_{n, \xi},
\]
(30)

hence (now we use Einstein’s notation for the sums),
\[
G_{m}^{\alpha} - G_{m}^{\alpha} \Sigma_{\xi, \xi'}^{\alpha} g_{\xi, \xi'} - G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi} + G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi},
\]
(31)

and
\[
G_{m}^{\alpha} - G_{m}^{\alpha} \Sigma_{\xi, \xi'}^{\alpha} g_{\xi, \xi'} - G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi} + G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi},
\]
(32)

so
\[
G_{m}^{\alpha} = G_{m}^{\alpha} \Sigma_{\xi, \xi'}^{\alpha} g_{\xi, \xi'} + G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi} + G_{n}^{\alpha} \Sigma_{n, \xi}^{\alpha} g_{n, \xi},
\]
(33)

where we define the renormalized Green functions \( \tilde{G}_{L}^{\alpha} \) for the left L electrode as
\[
g_{\xi, \xi'}^{\alpha} = G_{m}^{\alpha} \Sigma_{\xi, \xi'}^{\alpha} g_{\xi, \xi'}^{-1}.
\]
(34)

To solve for equation (33), we also need to know the matrix element \( G_{m}^{\alpha'} \):
hence,
\[ G_{\text{sh}_1}^{\prime} (1 - \Sigma_L^r \tilde{g}_L^r)_{\lambda, \lambda_1} = G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^r, \]  
(36)
so
\[ G_{\text{sh}_1}^{\prime} = G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^r, \]  
(37)
with a similar definition for the renormalized Green function \( \tilde{g}_L^r \) as given for \( \tilde{g}_L^l \) in equation (34). With our compact notation, we have
\[
\tilde{g}_L^{\prime/a} = \tilde{g}_L^{\prime/a} + \tilde{g}_L^{\prime/a} \Sigma_{L, \text{MB}, r/a} \tilde{g}_L^{\prime/a}.
\]  
(38)
Using the result of equation (37) into equation (33) and using the fact that \((1 - \Sigma_L^a \tilde{g}_L^a)^{-1} = (1 + \Sigma_L^a \tilde{g}_L^a)\), we find that
\[
G_{\text{sh}_1}^{\prime} = G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^r + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^l + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^r + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^l + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^{\prime} + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^{\prime} + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^{\prime} + G_{\text{sh}_1}^{\prime} \Sigma_{m, \lambda} \tilde{g}_{\text{sh}_1}^{\prime}
\]
\[
= (\alpha)(G_C \Sigma_{C, L} \tilde{g}_L^{\prime} )^{-1} \lambda, \]  
(39)
with
\[
\tilde{g}_L^{\prime} = \tilde{g}_L^{\prime} \Sigma_{L, \text{MB}, r/a} \tilde{g}_L^{\prime} + (1 + \tilde{g}_L^{\prime} \Sigma_{L, \text{MB}, r/a} \tilde{g}_L^{\prime}) \lambda, \]  
(40)
In other words: the \( \tilde{g}_L^{\prime} \) are the Green functions in the left \( L \) electrode renormalized by the many-body self-energy \( \Sigma_{L, \text{MB}, r/a} \) defined in the same subspace of the left \( L \) electrode. Similar results can be derived for the Green functions of the right \( R \) electrode.

4.2. The retarded Green function \( G'_C \) in the central region

We find for \( G'_C = \langle n | G' | m \rangle \)
\[
G'_C = \tilde{g}'_C + \tilde{g}'_C \Sigma_{C, \text{MB}, r/a} G'_C + \tilde{g}'_C \tilde{Y}'_{C, L+R, r} G'_C
\]
\[
= \left[ (\tilde{g}'_C)^{-1} - \Sigma_{C, \text{MB}, r/a} - \tilde{Y}'_{C, L+R, r} \right]^{-1}
\]
\[
= \left[ (\tilde{g}'_C)^{-1} - \tilde{Y}'_{C, L+R, r} \right]^{-1}, \]  
(41)
where \( \tilde{Y}'_{C, L+R, r} \) is the sum \( \tilde{Y}'_{C, L+R, r} = \tilde{Y}'_{C, L+R, r} + \tilde{Y}'_{C, L+R, r} \) of the generalized lead self-energies \( \tilde{Y}'_{C, r} \) \((\alpha = L, R)\) defined previously as \( \tilde{Y}'_{C, r} = (\Sigma_{\text{C}, \text{a}} \tilde{g}_r) \Sigma_{\text{a}, C} \) with \( \Sigma_{\text{C}, \text{a}} = \Sigma_{\text{C}, \text{a}} + \Sigma_{\text{C}, \text{MB}} \).

A similar expression can be derived for the advanced Green function \( G''_C \) in the central region by swapping \( r \leftrightarrow a \).

4.3. The lesser Green function \( G''_C \) in the central region

We find for \( G''_C = \langle n | G'' | m \rangle \) that
\[
G''_C = G'_C (\Sigma_{C, \text{MB}, r/a} + \tilde{Y}'_{C, L+R, r}) G'_C, \]  
(42)
with \( \tilde{Y}'_{C, L+R, r}(\omega) = \tilde{Y}'_{C, L+R, r}(\omega) + \tilde{Y}'_{C, L+R, r}(\omega) = \sum_{\alpha=L,R} \Sigma_{\text{C}, \text{a}}(\omega) \tilde{g}_r(\omega) \Sigma_{\text{a}, C}(\omega)), \) using the rules of analytical continuation for products given in appendix B, one gets \( \tilde{Y}'_{C, L+R, r} = \sum_{\alpha=L,R} \Sigma_{\text{C}, \text{a}} \tilde{g}_r(\omega) \Sigma_{\alpha, C} + \Sigma_{\text{C}, \text{a}} \tilde{g}_r(\omega) \Sigma_{\text{a}, C}. \)
4.4. The retarded Green function $G_{L,R}^r$ in the L and R lead

We find for $G_{L}^r = \langle \rho | G^r | \rho \rangle$ that

$$G_{\rho \rho'}^r = \tilde{g}_{\rho \rho'}^{r \prime} + \tilde{g}_{\rho \rho'}^{r \prime \prime} \tilde{Y}_{\rho \rho'}^{CL \prime},$$

where $\tilde{Y}_{\rho \rho'}^{CL \prime}$ is an embedding potential of the effects of the central region $C$ (connected to the left lead) on the right lead. It is defined as

$$\tilde{Y}_{\rho \rho'}^{CL \prime}(\omega) = \Sigma_{\rho \rho'}^{\prime}(\omega) \left[ \left[ \tilde{g}_{\rho \rho}^{C}(\omega) \right]^{-1} - \tilde{Y}_{C}^{L \prime}(\omega) \right]^{-1} \Sigma_{\rho \rho'}^{\prime}(\omega),$$

with $\Sigma_{\rho \rho'}^{\prime} = \Sigma_{\rho \rho'}^{RC} + \Sigma_{\rho \rho'}^{MB}$ and similarly for $\Sigma_{\rho \rho'}^{C}$. And $\left[ \left[ \tilde{g}_{\rho \rho}^{C}(\omega) \right]^{-1} - \tilde{Y}_{C}^{L \prime}(\omega) \right]^{-1}$ is a retarded Green function of the central region renormalized by the interaction inside $C$ and by the lead self-energy/embedding potential $\tilde{Y}_{C}^{L \prime}(\omega)$ of the left lead only, with $\tilde{g}_{\rho \rho}^{C}$ defined in equation (41) as $\left( \tilde{g}_{\rho \rho}^{C} \right)^{-1} = \left( \tilde{g}_{\rho \rho}^{C} \right)^{-1} - \Sigma_{\rho \rho}^{C}$.

Similarly we can find the expressions for the L lead Green function

$$G_{L}^{r} = \tilde{g}_{L}^{r} + \tilde{g}_{L}^{r \prime} \tilde{Y}_{L}^{C R \prime} G_{L}^{r},$$

$$\tilde{Y}_{L}^{C R \prime} = \Sigma_{L C}^{r} \left[ \left( \tilde{g}_{C}^{r \prime} \right)^{-1} - \tilde{Y}_{C}^{R \prime} \right]^{-1} \Sigma_{L C}^{r}.$$ 

Finally all the expressions given in this section hold for the advanced $G_{L,R}^{a}$ by swapping $r \leftrightarrow a$.

4.5. The lesser Green function $G_{L,R}^{<}$ in the leads

We first concentrate on $G_{L}^{<} = \langle G \Sigma g + g \rangle_{L}^{<}$. The calculations are rather lengthy, but somehow trivial, and include the derivation of many intermediate Green’s functions and many refactorizations. We find, in agreement with the results of the previous section, that

$$G_{L}^{<} = \left( 1 + G_{L}^{C} Y_{L}^{C R \prime} \right) \tilde{g}_{C}^{C} \left( 1 + Y_{L}^{C R \prime a} G_{L}^{a} \right) + G_{L}^{C} Y_{L}^{C C \prime} G_{L}^{<}$$

and

$$\tilde{Y}_{L}^{C R \prime} = \left( \Sigma_{L C}^{a} \tilde{g}_{C}^{a} \Sigma_{L C}^{a} \right)^{r \prime},$$

$$\tilde{g}_{C}^{C} = \left[ \left( \tilde{g}_{C}^{r \prime} \right)^{-1} - \tilde{Y}_{C}^{R \prime} \right]^{-1},$$

$$\tilde{g}_{C}^{R \prime} = \left( 1 + \tilde{g}_{C}^{R \prime a} Y_{C}^{R \prime a} \right) \tilde{g}_{C}^{C} \left( 1 + Y_{C}^{R \prime a} \tilde{g}_{C}^{a} \right) + \tilde{g}_{C}^{R \prime a} Y_{C}^{R \prime a} \tilde{g}_{C}^{a}.$$

The expression for $G_{L}^{<}$ can be obtained from equation (46) by swapping the index $L$ to $R$ and the self-energy $\tilde{Y}_{L}^{C R \prime}$ by $\tilde{Y}_{R}^{C L \prime}$ given in equation (44).

5. Current conservation condition

One of the most important physical properties that our formalism should obey is the current conservation condition. Before deriving the current conservation condition for the fully interacting system, we briefly recall the equivalent condition when the interactions are localized in the central region only.

5.1. Current conservation condition for the case of interaction only in the central region

Within the partitioned scheme devised by Meir and Wingreen, i.e. interaction only in the central region $C$, it can be shown that the trace

$$Tr_{a} \left[ \Sigma^{<}(\omega) G^{<}(\omega) \right] = 0$$

is zero.
vanishes for each \( \omega \), where \( \Sigma(\omega) \) is the total self-energy of the region \( C \): \( \Sigma = \Sigma^{MB}_C + \Sigma^{L}_C + \Sigma^{R}_C \). The \( \alpha \)-lead’s self-energy is \( \Sigma^\alpha = V_{Cu}g_\alpha V_{uC} \).

Equation (48) is derived from the definition \( G^{<}\Sigma^{<}\gamma(\omega) = G^{1}(\omega)\Sigma^{<}\gamma(\omega)G^{\alpha}(\omega) \) in the region \( C \), and hence \( \gamma^{-1}(\gamma - \Sigma^{<})\gamma^{\alpha} = \gamma^{<} = \gamma^{<} - \Sigma^{<} = \gamma^{<} - \Sigma^{<} = (\gamma^{\alpha})^{-1} - (\gamma')^{-1} \).

With equation (48), we can derive a condition that must be fulfilled by the interaction self-energy [48] in order to satisfy the current conservation condition \( I_L + I_R = 0 \) [48]. This condition is given by

\[
\int d\omega \; \text{Tr}_n \left[ \Sigma^{MB}_C^{<} G_C^{<} - \Sigma^{MB}_C^{>} G_C^{>} \right] = 0,
\]

which means that the integrated collision term must vanish. This is a condition familiarly obtained from a Boltzmann-like treatment of scattering theory [48]. When the interaction self-energy \( \Sigma^{MB} \) is derived from the so-called \( \Phi \)-derivable approximation [49, 50, 39, 40], it automatically satisfies the condition given by equation (49).

Equation (49) can also be used as a measure of the accuracy of numerical schemes used to calculate approximately the interaction self-energy. It can also be used as a general constraint equation in the determination a new functional forms for the interaction self-energy.

Now, when the interaction exists throughout the entire system, the derivation described above no longer holds and needs to be generalized to the presence of interaction within the leads and crossing at the left and right contacts.

5.2. Current conservation condition for the case of interaction everywhere

First we consider the general definition of the lesser and greater Green functions:

\[
G^{<} = (1 + G^{\gamma}\Sigma^{\gamma})(1 + \Sigma^{<}) + G^{\gamma}\Sigma^{<}\gamma^{\alpha}.
\]

The first term represents the initial conditions \( g^{<} \) before the interaction and the coupling between the different regions are applied.

For the central region, we have chosen the initial condition such as \( \langle n|g^{<}|m \rangle \equiv 0 \) (see equation (42)). We could have chosen another initial condition. Such choices have no effects on the steady-state regime when a steady current flows through the central region; however, the initial conditions play an important role in the transient behaviour of the current [51–54].

For the definition of the lesser left- and right-lead Green functions, however, it is not possible to neglect the initial conditions (before full interactions and coupling to the region central are taken into account). It would not be physically correct to ignore the presence of the left and right Fermi seas since they are the thermodynamical limit of the two semi-infinite leads, and act as an electron emitter and collector in our model of a device.

By using the standard Dyson equations for \( G^{\mu/\nu} \), we can recast equation (50) as

\[
G^{<} = G^{\gamma}\gamma^{\alpha} - \Sigma^{<}\gamma^{\alpha} G^{\gamma} = G^{\gamma}\Sigma^{<}\gamma^{\alpha} G^{\gamma} - G^{\gamma}\Sigma^{<}\gamma^{\alpha} G^{\gamma},
\]

with \( \bar{\Sigma}^{<} = \Sigma^{<} + \gamma^{<} \) and \( \gamma^{<} = (g^{\gamma})^{-1}g^{\gamma}(g^{\gamma})^{-1} \), and similarly for \( G^{>\gamma} \). Hence, \( \gamma^{<} - \gamma^{>\gamma} = (g^{\gamma})^{-1} - (g^{\gamma})^{-1} \) and \( \bar{\Sigma}^{<} - \Sigma^{<} = (G^{\gamma})^{-1} - (G^{\gamma'})^{-1} \). From these properties, it can be easily shown that

\[
\text{Tr}_{all}[(\bar{\Sigma}^{<}G^{<} - \Sigma^{<}G^{<})] = 0
\]

for each \( \omega \). The trace runs over all indices in the system all \( \equiv \{\lambda, n, \rho\} \) and the interaction \( \Sigma \) is spread over the whole \( L, C, R \) regions. This is a generalization of equation (48).

Because the trace runs over all the three subspaces, we can apply the usual cyclic permutation and recast equation (52) as follows:

\[
-\text{Tr}_{all}[(\Sigma G^{<} - \gamma^{<}\Sigma)G^{<}] + \text{Tr}_{all}[\gamma^{<}G^{<} - \gamma^{>\gamma}G^{<}] = 0
\]
or equivalently
\[
\int d\omega \text{Tr}_{\alpha \alpha}[(\Sigma G)^\omega - (G\Sigma)^\omega] + \text{Tr}_{\alpha \alpha}[\gamma^\omega G^\omega - \gamma^\omega G^\omega] = 0. \tag{54}
\]
Expanding the trace in the first term over each subspace \(\text{Tr}_{\alpha \alpha}[] = \text{Tr}_L[] + \text{Tr}_R[] + \text{Tr}_\ell[]\), one can easily identify the definition of the left \(I_L\) and right \(I_R\) currents from \(\text{Tr}_L[]\) and \(\text{Tr}_R[]\), respectively (see equation (9) above).

Hence, the condition of current conservation \(I_L + I_R = 0\) leads to
\[
\int d\omega \text{Tr}_{\alpha \alpha}[(\Sigma G)^\omega - (G\Sigma)^\omega] + \text{Tr}_{\alpha \alpha}[\gamma^\omega G^\omega - \gamma^\omega G^\omega] = 0. \tag{55}
\]
After further manipulation of the trace \(\text{Tr}_{\alpha \alpha}[]\) using the rules of analytical continuation and the relationship between the different Green functions and self-energies, we find that the current conservation implies that
\[
\int d\omega \text{Tr}_n[(\Sigma^{\text{MB}}_C + \hat{\Sigma}^{L+R}_C)^< G^\omega_c - (\Sigma^{\text{MB}}_C + \hat{\Sigma}^{L+R}_C)^< G^\omega_c] + \text{Tr}_{L,R}[\gamma^\omega G^\omega - \gamma^\omega G^\omega] = 0, \tag{56}
\]
where in the second trace the sum runs only over the left and right subspaces, because we have chosen the initial condition for the central region \(C\) such that \(\gamma^\omega < 0\).

What is really interesting with the first trace \(\text{Tr}_n[]\) in equation (56) is that it has exactly the same form as equation (52), but with all quantities (as well as the trace) defined within the central region \(C\) only (i.e. \(\hat{\Sigma} \equiv \Sigma^{\text{MB}}_C + \hat{\Sigma}^{L+R}_C\) in the region \(C\)). By looking at the definition of \(G^\omega_c\) given by equation (42), we can establish that, equivalently to equation (52), the trace actually vanishes:
\[
\text{Tr}_n[(\Sigma^{\text{MB}}_C + \hat{\Sigma}^{L+R}_C)^< G^\omega_c - (\Sigma^{\text{MB}}_C + \hat{\Sigma}^{L+R}_C)^< G^\omega_c] = 0 \tag{57}
\]
for each \(\omega\). Therefore, equation (56) reduces to
\[
\int d\omega \text{Tr}_{L,R}[\gamma^\omega G^\omega - \gamma^\omega G^\omega] = 0, \tag{58}
\]
a condition which however is almost systematically verified (see appendix C).

Hence, it is better to consider equation (57) to find the condition imposed by the current conservation. Indeed by treating each contribution in equation (57) separately and by integrating over the energy, we can introduce the definition of the currents \(I_L\) and \(I_R\) such as
\[
\int d\omega \text{Tr}_n[\Sigma^{\text{MB}}_C G^\omega_c - \Sigma^{\text{MB}}_C G^\omega_c] - i_L(\omega) + \Delta i_L(\omega) - i_R(\omega) + \Delta i_R(\omega) = 0, \tag{59}
\]
where \(I_n = e/h \int i_n(\omega)d\omega\) and \(\Delta i_n(\omega) = [\hat{\Sigma}^{\text{MB}}_C G^\omega_c - \hat{\Sigma}^{\text{MB}}_C G^\omega_c] + i_n(\omega).

Hence, the condition of current conservation \(I_L + I_R = 0\) leads to the final important result of this section:
\[
\int d\omega \text{Tr}_{n,L,C,R}[\Sigma^{\text{MB}}_a G^\omega_a - \Sigma^{\text{MB}}_a G^\omega_a] + \text{Tr}_n[\hat{\Sigma}^{L,L} G^\omega_c - (\hat{\Sigma}^{L,L}_c) G^\omega_c]
- (\hat{\Sigma}^{L,L}_c) G^\omega_c + (\hat{\Sigma}^{L,L}_c) G^\omega_c] + \text{Tr}_{n,L,C,R} [L \leftrightarrow R] = 0. \tag{60}
\]

Using the properties of the \(\hat{\Sigma}_C\) quantities (see section 3.3), we can rewrite the condition imposed by the current conservation as
\[
\int d\omega \text{Tr}_{n,L,C,R}[\Sigma^{\text{MB}}_a G^\omega_a - \Sigma^{\text{MB}}_a G^\omega_a] + \text{Tr}_n[\hat{\Sigma}^{L,L} G^\omega_c - (\hat{\Sigma}^{L,L}_c) G^\omega_c + (\hat{\Sigma}^{L,L}_c) G^\omega_c] + \text{Tr}_{n,L,C,R} [L \leftrightarrow R] = 0. \tag{61}
\]
To understand fully the conditions of current conservation, we make the following observations.

(i) Equation (61) is the generalization of equation (49) for the systems where the interaction spreads throughout. Like equation (49), it contains similar terms involving the left $L$ and right $R$ lead as well. But it also contains terms arising from the fact that the interaction is crossing at the $LC$ and $RC$ contacts. However, the physical interpretation of equation (61) still corresponds to the fact that the total integrated collision terms must vanish.

(ii) For interaction present only within the $C$ region, one can show that
\[
\tilde{\Upsilon}_{L}^{\alpha, \langle} C G \rangle_{\alpha} - \tilde{\Upsilon}_{L}^{\alpha, \rangle} C G \rangle_{\alpha} = 0
\]
as well as
\[
\tilde{\Upsilon}_{L}^{\alpha, \langle} C G \rangle_{\alpha} - \tilde{\Upsilon}_{L}^{\alpha, \rangle} C G \rangle_{\alpha} = 0
\]
since $\Sigma_{MB}^{\alpha} = V_{LC}$, and likewise for the terms involving the $RC$ interface. Furthermore, in that case, there are no interactions in the leads $\Sigma_{MB}^{\alpha} = 0$, and hence one recovers equation (49) as expected.

(iii) Equation (61) is also consistent with the one of the main point made in section 3.3: the current $I_{\alpha}$ ($\alpha = L$ or $R$) cannot be obtained from a trace over the central region defined as $Tr_{n}[Y_{\alpha, <} C G ] - Y_{\alpha, >} C G ]$. If it were the case, then the $\Delta i_{\alpha}(\omega)$ defined after equation (59) is
\[
\Delta i_{\alpha}(\omega) = \tilde{\Upsilon}_{\alpha, >} C G ] - \tilde{\Upsilon}_{\alpha, <} C G ] + i_{\alpha}(\omega) \equiv 0.
\]
And the current conservation condition would imply that equation (61) reduces to
\[
\int d\omega \; Tr_{n} = \lambda, \rho \left[ \Sigma_{\alpha}^{MB} G^{\alpha <} - \Sigma_{\alpha}^{MB} G^{\alpha >} \right] = 0.
\]
This equation concerns the collision terms within each of the three regions, but is not complete because it does not show any constraint on the interaction crossing at the $LC$ and $RC$ contacts.

6. Discussion and conclusion

In this paper, we have derived a complete and exact expression of the current crossing at the $LC$ (or $RC$) interface (defining the contact between the $L$ ($R$) lead and the central region $C$) for general systems with interaction both within each $L$, $C$, $R$ region and crossing at the left and right interfaces. Our result for the current equation (17) and equation (20) is general and obtained under only one approximation: there is no direct exchange and correlation effects between the left and right lead; a condition that is physically sound, especially for a large-ish central region where the spatial gap between the two electrodes is large enough so that the two electrodes interact only indirectly via the central region.

Our formalism includes all the cases previously studied with any kind of interactions present in the central region only [55–72]. It also includes other classes of problems such as those where interactions also exist within the leads but does not cross at the contacts [73]. Our formalism also provides a natural way to extend cases where the excitations exist in the leads and could cross at the contacts between the central region and the leads [74, 75].

We now discuss in more detail different open questions that are of importance for applications of our formalism to realistic systems.

6.1. Location of the interfaces

There is one arbitrary choice in our derivation: the location of the $LC$ and $RC$ interfaces with respect to the physical realistic system. Such locations are somehow arbitrary in our formalism but could be conveniently chosen for practical numerical calculations. We have already seen that, in some cases, a local quasi-equilibrium is reached within the left and right leads. In such cases, we get simplified results for the current, since the local non-equilibrium distribution functions $f_{L,R}^{eq}$, $f_{L,R}^{int}$ are equal to the local Fermi distribution in the left or right lead $f_{L,R} = f_{L,R}^{eq}$. 

15
6.2. The extended molecule

Our formalism provides a formal justification of the concept of the extended molecule that has been used so far within the conventional partitioned scheme with interaction present only in the C region. Being general, our formalism also provides the corresponding ‘correction’ terms needed when the interactions cross at the contacts and when the contacts are not in their respective local (quasi) equilibrium.

Our work also justifies the scheme recently used in [45] where two closed surfaces are used to define two sets of LC and RC interfaces around the molecule. Within the inner region, the electron–electron interaction is calculated via the GW scheme with the many-body self-energy \( \Sigma(\tau, \tau') = G(\tau, \tau') W(\tau, \tau') \). While the screened Coulomb interaction \( W = v + vPW \) and the polarization \( P \) are calculated for the extended region in order to ensure a better treatment of non-local screening effects. To some extent, this is an empirical way of defining the concept of generalized embedding potentials that we obtain in a formal manner in our formalism.

An extension of the present formalism to non-orthogonal basis sets as often used in electronic structure calculations with localized basis sets would potentially be useful. This has already been achieved for interaction present only in the central region by using a representation in the dual basis in which the lead subspaces are orthogonal to the central region subspace [30].

6.3. Generalized embedding potential

In a broader context, our formalism introduces in a formal manner the generalization of the concept embedding potential to interacting cases. In the case originally studied by Meir and Wingreen, where the interaction is present only in the central region, the effects of the leads on the Green functions defined with the subspace of the region \( C \) are taken into account via the so-called lead self-energies:

\[
\Sigma_{C}(\omega) = V_{C\alpha C}(\omega) \Sigma_{C}(\omega).
\]

These non-local self-energies are simply a matrix representation of the so-called embedding potential originally defined in real space by Inglesfield [41, 76, 77, 42, 43]. The latter can be seen as defining a surface (or two interfaces) around the central region that the interaction does not cross. The non-locality of the embedding potentials arises only from the Green functions defined on this surface.

In our formalism, when the interaction can cross the LC/RC interfaces, we obtain in a systematic way a generalization of the embedding potentials \( \tilde{Y}_{\alpha C}(\omega) \), defined as:

\[
\tilde{Y}_{\alpha C}(\omega) = \Sigma_{\alpha C}(\omega) \tilde{g}_{\alpha}(\omega) \Sigma_{\alpha C}(\omega).
\]

These generalized embedding potentials contain a ‘double’ non-locality, in the sense that the \( \Sigma_{\alpha C}^{MB} \) part of \( \Sigma_{\alpha C} \) can have a larger spatial extent than the hopping matrix elements \( V_{\alpha C} \). Hence the \( \tilde{Y}_{\alpha C} \) defines somehow not a simple surface but a ‘buffer’ zone that is contained between two surfaces whose separation is related to the characteristic (spatial decay) length of the interaction self-energies \( \Sigma_{\alpha C}^{MB} \equiv \Sigma_{\alpha C}(|x_a - x_n|) \).

6.4. Calculation of the self-energies

For practical numerical calculations of the current, one needs to choose the form for the interaction self-energies. They can be obtained from conventional many-body perturbation theory and Feynman diagramatics, extended onto the Keldysh contour. The interaction self-energy \( \Sigma^{MB} \) can be obtained from the \( \Phi \)-derivable conserving approximation [49, 50, 39, 40], and then they should automatically satisfy the condition of current conservation. We have given an example of such interaction self-energies in [35] for the case of electron–phonon coupling inside the region \( C \) and crossing at the LC interface. One could also devise other functional forms for the self-energies, such as the functional of the charge and spin densities,
and or of the current density itself. In these cases, one should devise the functionals such that the condition of current conservation is indeed fulfilled.

Finally, one should note that once the functional forms of the self-energies are chosen, one can perform the calculations self-consistently. The self-energies in the three regions $L, C, R$ and at the interfaces $LC$ and $RC$ are functionals of the other electron (and phonon) Green functions (or other physical quantities related to them such as the charge, spin or current density) defined inside the $L, C, R$ regions as well as at the two $LC$ and $RC$ interfaces. Hence the Green functions and self-energies need to be determined self-consistently in all the parts of the system in order to get the current of a fully many-body interacting nanojunction at non-equilibrium.

6.5. A special case for the self-energies

When modelling the self-energies such that $\tilde{\Upsilon}^{L,i}_C + (\tilde{\Upsilon}^{L,i}_C)^\dagger = 0$, we can express the current equation (17) as

$$I_L = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \text{Tr}_n \left[ \left( G^\omega_C - G^\omega_R \right) \tilde{\Upsilon}^{L,i}_C + G^\omega_C \left( \tilde{\Upsilon}^{L,i}_C - (\tilde{\Upsilon}^{L,i}_C)^\dagger \right) \right] + \text{Tr}_n \left[ \Sigma^\omega_{L}\rightarrow G^\omega_L - \Sigma^\omega_{L}\leftarrow G^\omega_L \right],$$

(63)

which bear even more resemblance to the Meir and Wingreen result, equation (28), and hence could be recast as a generalized Landauer-like expression for the current [14]. In such cases, the condition of current conservation becomes

$$\int d\omega \text{Tr}_{\omega=L,C,R} \left[ \Sigma^\omega_{\beta}\rightarrow G^\omega_{\beta} - \Sigma^\omega_{\beta}\leftarrow G^\omega_{\beta} \right] + \text{Tr}_n \left[ \left( \tilde{\Upsilon}^{L,i}_C - \tilde{\Upsilon}^{L,i}_L \right) G^\omega_C \right]$$

$$+ \text{Tr}_n \left[ \left( \tilde{\Upsilon}^{L,i}_C - \tilde{\Upsilon}^{L,i}_L \right) G^\omega_C \right] = 0.$$  

(64)

Equation (64) looks just like the sum of the integrated collision terms in the form of

$$\int d\omega \text{Tr}_\beta \left[ \Sigma^\omega_{\beta}\rightarrow G^\omega_{\beta} - \Sigma^\omega_{\beta}\leftarrow G^\omega_{\beta} \right] = 0,$$

(65)

where $\Sigma^\omega_{\beta}$ represents some interaction self-energy and the sum $\beta$ is over not only the three subspaces $L, C$ and $R$ but also the two interfaces $LC$ and $RC$.

By using the rules of analytical continuation and the relationships between the different Green functions, one can find that, in general, the sum $\tilde{\Upsilon}^{L,i}_C + (\tilde{\Upsilon}^{L,i}_C)^\dagger$ is given by

$$\tilde{\Upsilon}^{L,i}_C + (\tilde{\Upsilon}^{L,i}_C)^\dagger = \left( \Sigma^\omega_C \right)_{CL} + \Sigma^{\omega_C}_{LC} - \left( \Sigma^\omega_C \right)_{CL} + \Sigma^{\omega_C}_{LC} (\tilde{\Sigma})_{CL} - \Sigma^{\omega_C}_{LC} (\tilde{\Sigma})_{CL}.$$  

(66)

There are two different cases in which the sum $\tilde{\Upsilon}^{L,i}_C + (\tilde{\Upsilon}^{L,i}_C)^\dagger$ vanishes:

(i) when the interaction is only present in the central region. We have already discussed that case in length in the paper;

(ii) when interaction is instantaneous, i.e. local in time $\Sigma^\omega_{MB}(\tau, \tau') = v^\omega_{MB}(\tau) \delta(\tau - \tau')$. Hence, there are no lesser/greater components of the self-energy $\Sigma^\omega_{MB,>\leftarrow} = 0$. This occurs, as already discussed, in mean-field-based and in density-functional-based theories for which a single (quasi-)particle description of the system is available.

Finally, it would be interesting to study and find cases which go beyond mean-field-based or density-functional-based methods, and for which $\tilde{\Upsilon}^{L,i}_C + (\tilde{\Upsilon}^{L,i}_C)^\dagger = 0$. If such cases exist, it would still be possible to analyse their transport properties in terms of a generalized Landauer-like approach [14].
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Appendix A. Relationships between Green’s functions

By definition, the complex conjugation of the different Green functions follows the rules:

\[ G^c(1, 2) = (G^c(2, 1))^* \]
\[ G^\approx(1, 2) = -(G^\approx(2, 1))^*. \]

Similar expressions also hold for the self-energies \( \Sigma \).

Furthermore, there exist relationships between the different components of the Green functions (or self-energies) on the Keldysh time-loop contour \( C_K \). They are given by

\[ X^r = X^{++} - X^{-+} = X^{+-} - X^{--} \]
\[ X^a = X^{++} - X^{-+} = X^{+-} - X^{--} \]
\[ X^{++} + X^{--} = X^{++} + X^{--} \]
\[ X^{++} - X^{--} = X^{---} - X^{--} \]
\[ \text{(A.1)} \]

with \( X^{i\eta_1}(12) \equiv G^{i\eta_2}(12) \) or \( \Sigma^{i\eta_2}(12) \), and where \( (i = 1, 2) \) is the composite index for spacetime location \((x, t_i)\) and \( \eta_i \) is the index of the Keldysh time-loop contour \( C_K \) branch (+ forward time arrow, − backward time arrow) on which the time \( t_i \) is located. The conventional lesser and greater projections are defined, respectively, as \( X^< \equiv X^{++} \) and \( X^> \equiv X^{--} \), and the usual time-ordered (anti-time-ordered) as \( X^t \equiv X^{++} \) (\( X^\tilde{t} \equiv X^{--} \)).

Appendix B. Rules for analytical continuation

For the following products \( P_{(i)}(\tau, \tau') \) on the time loop contour \( C_K \),

\[ P_{(2)} = \int_{C_K} AB, \]
\[ P_{(3)} = \int_{C_K} ABC, \]
\[ P_{(n)} = \int_{C_K} A_1 A_2 ... A_n, \]

we have the following rules for the different components \( P_{(i)}^x(t, t') \) on the real time axis: (\( x = r, a, >, < \))

\[ P_{(2)}^c = \int_t A^c B^c + A^\approx B^d, \]
\[ P_{(3)}^c = \int_t A^\approx B^c C^d + A^c B^\approx C^d + A^d B^c C^<, \]
\[ P_{(n)}^r = \int_t A_1^r A_2^r ... A_n^r, \]
\[ P_{(n)}^a = \int_t A_1^a A_2^a ... A_n^a. \]
Appendix C. Proof that $\int d\omega \, \text{Tr}_{L,R} \left[ \gamma^x G^\omega - \gamma^z G^\omega \right] = 0$

From the definition $\gamma^x(\omega) = (g^x)^{-1} g^x(\omega) (g^x)^{-1}$, the quantities $\gamma^x$ have only matrix elements within the $\alpha = L, R$ lead since they involve only the non-interacting Green functions. Consequently, we only have to prove that

$$\int d\omega \, \text{Tr}_{\alpha=L,R} \left[ \gamma^\omega_{\alpha} G^\omega_{\alpha} - \gamma^\omega_{\alpha} G^\omega_{\alpha} \right] = 0.$$  \hfill (C.1)

We now introduce the non-equilibrium distribution $f^{\alpha>\omega}(\omega)$ and $f^{\alpha<\omega}(\omega)$ defined, in the $\alpha$ lead subspace, from the generalized Kadanoff–Baym ansatz [44] as follows:

$$G^\omega_{\alpha}(\omega) = f^{\alpha>\omega}(\omega) g^\omega_{\alpha}(\omega) - g^\omega_{\alpha}(\omega) f^{\alpha<\omega}(\omega),$$

$$G^\omega_{\text{R}}(\omega) = f^{\alpha>\omega}(\omega) G^\omega_{\alpha}(\omega) - G^\omega_{\alpha}(\omega) f^{\alpha<\omega}(\omega),$$  \hfill (C.2)

with $\omega = \omega$. The distribution function $f^{\alpha>\omega}$ is defined for the non-interacting and uncoupled lead $\alpha$, and is given by the Fermi distribution of the lead $\alpha$ at its own equilibrium. Using these definitions, we can reformulate equation (C.1) after further manipulation as

$$\text{Tr}_{L,R} \left[ \gamma^x G^\omega - \gamma^z G^\omega \right] = (2\pi)^2 \text{Tr}_{L,R} \left[ f^{\alpha>\omega} B_{\alpha} A^G_{\alpha} - f^{\alpha<\omega} A^G_{\alpha} B_{\alpha} \right]$$

$$= (2\pi)^2 \text{Tr}_{L,R} \left[ (f^{\alpha>\omega} - f^{\alpha<\omega}) A^G_{\alpha} B_{\alpha} \right],$$  \hfill (C.3)

where

$$A^G_{\alpha}(\omega) = (G^\omega_{\alpha}(\omega) - G^\omega_{\text{R}}(\omega)) / 2\pi i,$$

$$B_{\alpha}(\omega) = (g^\omega_{\alpha}(\omega))^{-1} - (g^\omega_{\text{R}}(\omega))^{-1} = ((g^\omega_{\alpha}(\omega))^{-1} - (g^\omega_{\text{R}}(\omega))^{-1}) / 2\pi i.$$  \hfill (C.4)

In the second equality of equation (C.3), we have used a diagonal representation for the non-equilibrium distributions $f^{\alpha>\omega}$ and $f^{\alpha<\omega}$.

There are several different cases for which equation (C.1) vanishes.

(i) Following the same reasoning as in section 3.4, when the LC interfaces are located well inside the lead $L$, the corresponding states are in their local equilibrium and $f^{\alpha>\omega} - f^{\alpha<\omega} \sim 0$.

(ii) Following the definition $B_{\alpha} = ((g^\omega_{\alpha}(\omega))^{-1} - (g^\omega_{\text{R}}(\omega))^{-1}) / 2\pi i = ((\omega - H_{\text{L}} + i\eta) - (\omega - H_{\text{L}} - i\eta)) / 2\pi i = \eta i / \pi \sim 0$. Therefore, equation (C.3) vanishes unless $A^G_{\alpha}(\omega)$ is singular at some energy. This would correspond to the appearance of localized bound states in the $\alpha$ lead induced by the interaction (and/or by the non-equilibrium condition). Although such an appearance cannot be ruled out in principle, it seems to correspond to pathological cases not relevant for the description of the metallic leads used in the experiments.

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