Dictionary between scattering matrix and Keldysh formalisms for quantum transport driven by time-periodic fields.

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We present the relation between the Floquet scattering matrix and the non-equilibrium Green's function formalisms to transport theory in noninteracting electronic systems in contact to reservoirs and driven by time-periodic fields. We present a translation formula that expresses the Floquet scattering matrix in terms of a Fourier transform of the retarded Green's function. We prove that such representation satisfies the fundamental identities of transport theory. We also present the "adiabatic" approximation to the dc-current in the language of the Keldysh formalism.

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I. INTRODUCTION

In the last years, there has been an increasing theoretical and experimental activity around quantum transport phenomena induced by time-dependent fields. Pumping phenomena in mesoscopic systems constitutes a very interesting case, where periodic out-of-phase potentials deform the gates of semiconductor structures allowing for the generation of dc-currents even in the absence of a static bias.[1,2,3,4,5,6,7,8,9,10,11,12,13,14]

The scattering matrix approach and Keldysh nonequilibrium Green's function technique are the most powerful formalisms in the theory of quantum transport. Recently, the generalization of the Scattering (S) Matrix theory to time-periodic transport phenomena in an energy representation has been formulated[15,16,17], while an alternative treatment in a time representation has been proposed in Refs. 18,19. Keldysh formalism as a theoretical tool to investigate time-dependent transport phenomena in mesoscopic systems has been introduced some time ago[20,21] and has been employed to study problems like ac-transport through quantum dots[22] and superlattices[23], Josephson junctions[24,25] and quantum pumps[26,27]. Recently a practical formulation to treat problems with harmonically time-dependent potentials has been presented and used to investigate quantum transport in a mesoscopic ring threaded by a time-dependent flux[28] and systems with ac-potentials[29,30]. Other formalisms to describe quantum transport in the presence of time-periodic fields are based in a modified transfer matrix approach[31] and in the Floquet representation of the Hamiltonian with the introduction of non-hermitian dynamics for the wave function propagation, in order to represent dissipative effects.[32,33,34]

The Scattering Matrix formalism is basically a single-particle approach. Therefore, it cannot be directly applied to systems described by Hamiltonians containing many-particle interactions. The theoretical framework in which Keldysh formalism is based is exactly the opposite one, namely the systematic treatment of many-particle interacting systems. This formalism is, however, also adequate to investigate transport phenomena through mesoscopic systems even in the case that many-body interactions do not play a relevant role. The reason it that the effect of the environment, in particular, the leads and reservoirs to which the mesoscopic system is connected, are suitably represented in terms of self-energies. In the description of quantum transport in systems of non-interacting electrons, the agreement between both formalisms is expected to be the rule. In the context of stationary transport, the equivalence between the two approaches was first pointed out by Fisher and Lee.[35]

An important experimental situation corresponds to the case of slowly oscillating driving fields. The low frequency regime is sometimes loosely referred to as "adiabatic". This word stems from the Greek word "a-diabatos", which means "not passable". Traditionally, in theoretical physics, this term is employed when an isolated or closed quantum mechanical system is perturbed by a time-dependent Hamiltonian in such a way that the eigenstates do not mix as time evolves. This idea cannot be trivially exported to describe a quantum system coupled to an environment where the spectrum is continuum and concepts like energy levels are not well defined. In the framework of open quantum systems, the term "adiabatic" is sometimes understood as a synonymous of low frequency behavior while it is also sometimes employed to define a description where the variable t in the time-dependent piece of the Hamiltonian is considered as a frozen parameter. An important number of works have been devoted to investigate quantum transport in pumps within the low-frequency regime. In particular, an "adiabatic" approximation to the Floquet scattering matrix has been introduced[5,6,13,15,16,17] which, in practice, allows for the evaluation of the contribution to the pumped dc-current that behaves linearly in the driving frequency.

The aim of this work is twofold. On one hand, we show that, for non-interacting quantum systems driven by time-periodic fields, in contact to static reservoirs with arbitrary densities of states, or with oscillating reservoirs described by smooth densities of states, it is possible to establish a transparent and complete dictionary between the Floquet scattering matrix approach of Refs. 15,16,17 and the Keldysh Green's function treatment of Ref. 29. The second goal of this work is to formulate an "adiabatic" approximation, analogous to the one used in scattering matrix formalism, in the language of nonequilibrium Green's functions.

The work is organized as follows. In section II we summarize the description of quantum transport within the scattering matrix approach as well as the "adiabatic" approximation to the Floquet scattering matrix. The description of quantum transport for non-interacting electrons driven by time-periodic fields in the framework of Keldysh formalism is summarized in section III. We present several equivalent equations to evaluate the dc-component of the current flowing between the reservoirs and the central mesoscopic driven system. We consider cases where the pumping voltages are locally applied only at the central system, as well as cases where the voltages are applied at the reservoirs. A formula that allows for the translation between the two formalisms is presented in section IV. In section V we show that a fundamental property like the unitarity of the Floquet S-matrix can be proved in terms of identities satisfied by the non-equilibrium Green's functions. In section VI we present the adiabatic approximation formulated in the language of non-equilibrium Green's functions. Finally, section VII is devoted to summary and conclusions. We have also included appendices A, B, C, D and E with relevant identities and properties used along the work.

II. SCATTERING MATRIX FORMALISM

A. General formalism

The scattering matrix approach to quantum transport, usually referred to as the Landauer-Büttiker approach,[36,37] considers the propagation of carriers through a mesoscopic sample as a scattering process. The sample (scatterer) is assumed to be connected to several N_r contacts (playing the role of electron reservoirs) via single channel leads. Then, all the information about transport properties of a mesoscopic sample is encoded in the scattering matrix $\hat{S}$ whose elements are quantum mechanical amplitudes for electrons coming from some lead to be scattered into the same or any other lead. These amplitudes are normalized in such a way that their square define the corresponding particle fluxes (currents).

In each lead there are two kinds of states, incoming to and outgoing off the scatterer. Correspondingly, we introduce two kinds of second-quantization operators $\hat{a}_\alpha(E)/\hat{a}^\dagger_\alpha(E)$ and $\hat{b}_\alpha(E)$ /$\hat{b}^\dagger_\alpha(E)$ which annihilate/create one particle in the lead α with energy E. Using these operators one can calculate a time-dependent current flowing into lead α as follows (we use a convention that the current directed from the scatterer towards the reservoir is positive):[37]

$$
\begin{aligned}
I_\alpha(t) = \frac{e}{h}\int_0^\infty\int_0^\infty dE dE' e^{i\frac{E-E'}{\hbar}t} \\
\times\left\{\langle\hat{b}^\dagger_\alpha(E)\hat{b}_\alpha(E')\rangle - \langle\hat{a}^\dagger_\alpha(E)\hat{a}_\alpha(E')\rangle\right\}.
\end{aligned} \tag{1}
$$

Here $\langle\dots\rangle$ means quantum-statistical averaging over equilibrium states of all the reservoirs which are assumed to be unaffected by the coupling to the scatterer.

1. *Time-periodic local potentials and static reservoirs*

The particles incoming from some reservoir α are equilibrium particles. Therefore, if the reservoirs are stationary we have:

$$
\langle\hat{a}^\dagger_\alpha(E)\hat{a}_\beta(E')\rangle = \delta_{\alpha\beta}\delta(E-E')f_\alpha(E), \tag{2}
$$

where $f_\alpha(E)$ is the Fermi distribution function for electrons in reservoir α. In general, the reservoirs have different chemical potentials μ_α and temperatures T_α. The oscillating potentials at reservoirs will be considered separately.

The operators $\hat{b}_\alpha$ for particles outgoing (i.e., scattered) into the lead α are related to the operators $\hat{a}_\beta$ for incoming particles ($\beta = 1,\dots,N_r$) through the scattering matrix.[37] In the present paper we will consider the scatterer which is driven by external forces that are periodic in time with period $\tau_0 = 2\pi/\Omega_0$. Interacting with such a scatterer an electron can gain or loss some energy quanta $n\hbar\Omega_0$, $n = 0,\pm1,\dots$ Therefore, in this case the elements $S_{F,\alpha\beta}(E_n, E)$ of the scattering matrix (the Floquet scattering matrix $\hat{S}_F$, see, e.g., Ref.38) are photon-assisted amplitudes (times $\sqrt{k_n/k}$, $k = \sqrt{2mE/\hbar^2}$) for an electron with energy E entering the scatterer through lead β and to leave the scatterer with energy $E_n = E + n\hbar\Omega_0$ through lead α. Then the desired relation between operators $\hat{b}$ for outgoing particles and $\hat{a}$ for incoming particles reads as follows:[15]

$$
\hat{b}_\alpha(E) = \sum_{\beta=1}^{N_r}\sum_n S_{F,\alpha\beta}(E, E_n)\hat{a}_\beta(E_n). \tag{3}
$$

The sum over n runs over those n for which $E_n > 0$. In general, some elements of the Floquet scattering matrix describe transitions between the bound states ($E_n < 0$) and propagating (i.e., current-carrying) states or vice versa. Such processes do not contribute to Eq.(3). Therefore, in what follows, by the Floquet scattering matrix we will mean the submatrix corresponding to transitions between propagating states only. In fact, if $\hbar\Omega_0 \ll E$, the sum in Eq.(3) runs over all the integers: $-\infty < n < \infty$. Note that if the scatterer is stationary, then only the term with $n = 0$ remains non-vanishing.

Current conservation implies that the Floquet scattering matrix is a unitary matrix:[15,16]

$$\sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} S^*_{\beta\alpha}(E_n, E) S_{\beta\gamma}(E_n, E_m) = \delta_{m0}\delta_{\alpha\gamma}, \tag{4a}$$

$$\sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} S^*_{\alpha\beta}(E, E_n) S_{\gamma\beta}(E_m, E_n) = \delta_{m0}\delta_{\alpha\gamma}. \tag{4b}$$

One can easily check that the unitary conditions guarantee that the operators for outgoing particles obey the same anti-commutation relations as the operators for incoming particles:

$$\begin{aligned} [\hat{a}^\dagger_\alpha(E), \hat{a}_\beta(E')] &= \delta_{\alpha\beta}\delta(E - E'), \\ [\hat{b}^\dagger_\alpha(E), \hat{b}_\beta(E')] &= \delta_{\alpha\beta}\delta(E - E'). \end{aligned} \tag{5}$$

However, in contrast to incoming particles, the scattered ones are non-equilibrium particles with the distribution function $f^{(out)}_\alpha(E)\delta(E - E')\delta_{\alpha\beta} = \langle \hat{b}^\dagger_\alpha(E)\hat{b}^\dagger_\beta(E')\rangle$ being different from the Fermi distribution function:[15]

$$f^{(out)}_\alpha(E) = \sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} \left|S_{F,\alpha\beta}(E, E_n)\right|^2 f_\alpha(E_n). \tag{6}$$

Using Eqs.(2) and (3) one can calculate the time-dependent current $I_\alpha(t)$, Eq.(1), flowing into the lead α. The dc component I_α of this current reads as follows:

$$I_\alpha = \frac{e}{h}\int_0^\infty dE \left\{ f^{(out)}_\alpha(E) - f_\alpha(E)\right\}. \tag{7}$$

Substituting Eq.(6) into the above equation, using Eq.(4b) and making the shift $E \to E - n\hbar\Omega_0$ we finally get:

$$\begin{aligned} I_\alpha = \frac{e}{h}\int_0^\infty dE \sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} &\left|S_{F,\alpha\beta}(E_n, E)\right|^2 \\ &\times \left\{ f_\beta(E) - f_\alpha(E_n)\right\}. \end{aligned} \tag{8}$$

This expression emphasizes that for weak driving amplitudes and small frequencies, only electrons close to the Fermi level do contribute to the current.

An alternative expression for the above current may be obtained by making the energy shift in $f^{(out)}_\alpha(E)$ only and using Eq.(4a). We get a dc current in a more usual form (as a difference of forward and back photon-assisted transmission probabilities):

$$\begin{aligned} I_\alpha = \frac{e}{h}\int_0^\infty dE \sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} \Big\{ &\left|S_{F,\alpha\beta}(E_n, E)\right|^2 f_\beta(E) \\ &- \left|S_{F,\beta\alpha}(E_n, E)\right|^2 f_\alpha(E)\Big\}. \end{aligned} \tag{9}$$

Given the above equations either (8) or (9) define a dc current flowing through the scatterer coupled to stationary equilibrium reservoirs.

2. *Time-dependent voltages at the reservoirs*

If the reservoirs are subject to oscillating voltages with the same frequency:

$$V_\alpha(t) = V_\alpha \cos(\Omega_0 t + \varphi_\alpha), \tag{10}$$

then we proceed as follows.[16,39] Within the reservoir with uniform oscillating potential the electron wave function has the structure of the Floquet function type:

$$\begin{aligned} \Psi_\alpha(V_\alpha, E, \mathbf{r}) &= e^{-iEt/\hbar - i\hbar^{-1}\int_{-\infty}^{t} dt' eV_\alpha(t')}\psi_E(\mathbf{r}) \\ &= e^{-iEt/\hbar}\psi_E(\mathbf{r})\sum_{n=-\infty}^{\infty} J_n\left(\frac{eV_\alpha}{\hbar\Omega_0}\right) e^{-in(\Omega_0 t + \varphi_\alpha)}. \end{aligned} \tag{11}$$

We introduce operators $\hat{a}'^\dagger(E)/\hat{a}'(E)$ which create/annihilate one particle in the given above Floquet state. The corresponding distribution function is the Fermi distribution function: $\langle \hat{a}'^\dagger_\alpha(E)\hat{a}'_\beta(E')\rangle = \delta_{\alpha\beta}\delta(E - E')f_\alpha(E)$, where the Floquet quasi-energy E is chosen to be equal to the energy of the stationary state with the same spatial part $\psi_E(\mathbf{r})$. This follows from the fact that the uniform oscillating potential does not change the normalization of the wave function: $\int d^3r|\Psi(E)|^2 = \int d^3r|\psi_E|^2 = 1$. As a consequence, the only occupied states $\Psi(E)$ are those that correspond to the ones in the stationary reservoir with the same ψ_E.

Then we construct operators $\hat{a}_\alpha(E)/\hat{a}^\dagger_\alpha(E)$ corresponding to incoming particles in the leads with definite energy E as follows:

$$\hat{a}_\alpha(E) = \sum_{n=-\infty}^{\infty} J_n\left(\frac{eV_\alpha}{\hbar\Omega_0}\right) e^{-in\varphi_\alpha}\hat{a}'_\alpha(E - n\hbar\Omega_0). \tag{12}$$

The operators $\hat{b}$ for scattered particles are related to the operators $\hat{a}$ for incoming particles through the scattering matrix of the sample, Eq.(3). Substituting the calculated $\hat{a}$ and $\hat{b}$ operators into Eq.(1) and averaging over the time-period we get a dc current in the presence of oscillating potentials $V_\alpha(t)$ at reservoirs as follows:

$$\begin{aligned} I_\alpha = \frac{e}{h}\int_0^\infty dE \sum_{n=-\infty}^{\infty} \Bigg\{ &\sum_{\beta=1}^{N_r} f_\beta(E - n\hbar\Omega_0) \\ &\times \sum_{m,q=-\infty}^{\infty} S^*_{F,\alpha\beta}(E, E_q) S_{F,\alpha\beta}(E, E_m) \\ &\times J_{n+q}\left(\frac{eV_\beta}{\hbar\Omega_0}\right) J_{n+m}\left(\frac{eV_\beta}{\hbar\Omega_0}\right) e^{i(q-m)\varphi_\beta} \\ &- f_\alpha(E - n\hbar\Omega_0) J_n^2\left(\frac{eV_\alpha}{\hbar\Omega_0}\right)\Bigg\}. \end{aligned} \tag{13}$$

Using Eq.(4b) and making the shift $E \to E + n\hbar\Omega_0$ in the last term one can rewrite the above equation in a more convenient form:

$$I_\alpha = \frac{e}{\hbar} \int_0^\infty dE \sum_{n=-\infty}^{\infty} \sum_{\beta=1}^{N_r} \Big\{ f_\beta(E - n\hbar\Omega_0) - f_\alpha(E) \Big\}$$
$$\times \sum_{m,q=-\infty}^{\infty} S^*_{F,\alpha\beta}(E, E_q) S_{F,\alpha\beta}(E, E_m)$$
$$\times J_{n+q}\left(\frac{eV_\beta}{\hbar\Omega_0}\right) J_{n+m}\left(\frac{eV_\beta}{\hbar\Omega_0}\right) e^{i(q-m)\varphi_\beta}. \tag{14}$$

To calculate the current flowing through the driven mesoscopic sample it is necessary to know the Floquet scattering matrix $\hat{S}_F$. At strong driving this matrix has an infinite number of elements. Therefore, its calculation is, in practice, a non-trivial problem. This problem can be greatly simplified if the driving frequency is small. In this limit the Floquet scattering matrix $\hat{S}_F$ can be related to the stationary scattering matrix $\hat{S}_0$ having much less number of elements.

B. Adiabatic approximation

At low driving frequencies, $\Omega_0 \to 0$, one can expand the elements of the Floquet scattering matrix in powers of Ω_0. The lowest-order terms read as follows:[17]

$$\hat{S}_F(E_n, E) = \hat{S}_{0,n}(E) + \frac{n\hbar\Omega_0}{2} \frac{\partial \hat{S}_{0,n}(E)}{\partial E} + \hbar\Omega_0 \hat{A}_n(E) + \mathcal{O}(\Omega_0^2), \tag{15a}$$

$$\hat{S}_F(E, E_n) = \hat{S}_{0,-n}(E) + \frac{n\hbar\Omega_0}{2} \frac{\partial \hat{S}_{0,-n}(E)}{\partial E} + \hbar\Omega_0 \hat{A}_{-n}(E) + \mathcal{O}(\Omega_0^2). \tag{15b}$$

Here $\hat{S}_{0,n}$ is the Fourier transform for the frozen scattering matrix which is defined as follows:

$$\hat{S}_0(E, t) = \sum_{n=-\infty}^{\infty} e^{-in\Omega_0 t} \hat{S}_{0,n}(E). \tag{16}$$

Let the stationary scattering matrix $\hat{S}_0(E)$ depend on some parameters $p_i \in \{P\}, i = 1, 2, \dots, N_p$ which are varied under an external drive. Since we assume that the latter is periodic, the parameters are periodic in time as well, $p_i(t + \tau_0) = p_i(t)$. The frozen scattering matrix $\hat{S}_0(E, t)$ is defined as the stationary scattering matrix $\hat{S}_0(E, \{P\})$ with parameters being dependent on time: $\hat{S}_0(E, t) = \hat{S}_0(E, \{P(t)\})$. We emphasize that the frozen scattering matrix does not define the scattering properties of a driven scatterer. Only the Floquet scattering matrix does.

The matrix $\hat{A}(E, t)$, whose Fourier elements $\hat{A}_n(E)$ that enters the expansion (15), cannot be related to the stationary scattering matrix and have to be calculated independently, see Ref.17 for simple examples. Notice that the current conservation introduces some constraints to the matrix $\hat{A}$. Substituting Eq.(15) into Eq.(4) and taking into account that the stationary scattering matrix is unitary we get the following:[16]

$$\hbar\Omega_0 \Big\{ \hat{S}_0^\dagger \hat{A} + \hat{A}^\dagger \hat{S}_0 \Big\} = \frac{i\hbar}{2} \left(\frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E} - \frac{\partial \hat{S}_0^\dagger}{\partial E} \frac{\partial \hat{S}_0}{\partial t} \right). \tag{17}$$

The matrix $\hat{A}$ reflects a directional asymmetry of a dynamical scattering process arising as a result of interference of photon-assisted scattering amplitudes.[40]

Equations (15) and (17) show that the expansion in powers of Ω_0 is, in fact, an expansion in powers of $\hbar\Omega_0/\delta E$, where δE is an energy scale characteristic for the stationary scattering matrix. The energy scale δE relates to the inverse time spent by an electron inside the scattering region (the dwell time). Therefore, alternatively one can say that the adiabatic expansion given in Eq.(15), can be applied if the period of an external drive is large compared with the dwell time. This definition of an adiabatic regime is different from a usually used in quantum mechanics one which relates the excitation quantum $\hbar\Omega_0$ to the electron level spacing.

We conclude, to find the Floquet scattering matrix with accuracy of order Ω_0 it is necessary to calculate two matrices, $\hat{S}_0(E, t)$ and $\hat{A}(E, t)$, each of them having $N_r \times N_r$ elements. If this is done we can calculate the current up to terms of order Ω_0. For the simplicity we suppose that all the reservoirs have the same chemical potentials and temperatures, hence $f_\alpha(\omega) = f_0(\omega), \forall\alpha$. Then substituting Eq.(15) into Eq.(14), expanding the difference of Fermi functions in powers of Ω_0, performing inverse Fourier transformation, and keeping at the end only linear in Ω_0 and $V_\alpha(t)$ terms we get the dc current as a sum of three contributions:

$$I_\alpha = \int_0^\infty dE \left(-\frac{\partial f_0(E)}{\partial E} \right) \int_0^{\tau_0} \frac{dt}{\tau} \Big\{ I_\alpha^{(pump)}(E, t) + I_\alpha^{(rect)}(E, t) + I_\alpha^{(int)}(E, t) \Big\}, \tag{18a}$$

$$I_\alpha^{(pump)}(E, t) = -i \frac{e}{2\pi} \left(\hat{S}_0(E, t) \frac{\partial \hat{S}_0^\dagger(E, t)}{\partial t} \right)_{\alpha\alpha}, \tag{18b}$$

$$I_\alpha^{(rect)}(E, t) = \frac{e^2}{h} \sum_{\beta=1}^{N_r} \Big\{ V_\beta(t) - V_\alpha(t) \Big\} \Big| S_{0,\alpha\beta}(E, t) \Big|^2, \tag{18c}$$

$$I_\alpha^{(int)}(E, t) = \frac{e^2}{h} \sum_{\beta=1}^{N_r} V_\beta(t) \Big\{ 2\hbar\Omega_0 \mathrm{Re}\big[S^*_{0,\alpha\beta}(E, t) A_{\alpha\beta}(E, t) \big] + \frac{i\hbar}{2} \left(\frac{\partial S_{0,\alpha\beta}}{\partial t} \frac{\partial S^*_{0,\alpha\beta}}{\partial E} - \frac{\partial S_{0,\alpha\beta}}{\partial E} \frac{\partial S^*_{0,\alpha\beta}}{\partial t} \right) \Big\}. \tag{18d}$$

Here, in Eq.(18d), we have integrated over energy the term proportional to $\partial^2 f_0/\partial E^2$ and made it to be proportional to $\partial f_0/\partial E$.

The first contribution, $I_\alpha^{(pump)}(E,t)$, is an adiabatic current pumped by a dynamical scatterer.[6] This current is non zero if the time-reversal symmetry in the system is broken by the external drive, $\hat{S}_0(t) \neq \hat{S}_0(-t)$. To this end at least two parameters of the scatterer have to be varied with a phase lag different from zero and π. The second contribution, $I_\alpha^{(rect)}(E,t)$, is due to the rectification of ac currents flowing under the influence of ac voltages by the varying conductance of a sample.[41] This contribution is non-zero if the potentials $V_\alpha(t)$ are different. The third contribution, $I_\alpha^{(int)}(E,t)$, is due to interference between the ac currents generated by the dynamical scatterer and the ac currents produced by the external voltages.[16] This current can be non-zero even if all the potentials $V_\alpha(t)$ are the same. Formally, this contribution can be viewed as due to external voltages acting as additional pumping parameters. So, if all the potentials are the same, $V_\alpha(t) = V(t), \forall\alpha$ and only one parameter of a scatterer is varied then only the third contribution remains.

Now, we turn to the Keldysh formalism to quantum transport for harmonically driven systems and then, we will establish a correspondence between the two formalisms.

III. QUANTUM TRANSPORT WITHIN KELDYSH FORMALISM

A. Hamiltonian, Green's functions and Dyson equations

The goal of Keldysh formalism is the evaluation of the Green's function of the system in the real time axis. The starting point is a Hamiltonian to describe the driven system in contact to the N_r particle reservoirs through connecting leads:

$$H(t) = H^{sys}(t) + H^{cont} + H^{res}(t). \tag{19}$$

Although this formalism provides a systematic way to approximately treat many-body interactions, we focus in Hamiltonians corresponding to non-interacting electrons, which can be treated exactly. In several problems, it is convenient to describe the central driven system by a lattice model containing N sites. We adopt here that point of view. For such a system a generic Hamiltonian of spinless noninteracting electrons reads

$$H^{sys}(t) = \sum_{l,l'=1}^{N} (H_{l,l'}^{sys}(t) c_l^\dagger c_{l'} + H.c.). \tag{20}$$

We assume that the matrix elements contain static and time-dependent pieces of the form: $H_{l,l'}^{sys}(t) = \varepsilon_{l,l'}(\Phi) + V_{l,l'}(t,\delta_{l,l'})$, being Φ a static magnetic flux and the terms depending on the driving fields being periodic in time, $V_{l,l'}(t,\delta_{l,l'}) = \sum_{k=-\infty}^{\infty} e^{-ik\Omega_0 t} V_{l,l'}(k)$ with amplitudes depending on the phases $\delta_{l,l'}$ and $V_{l,l'}(0) = 0$. For the moment, we do not write explicitly the dependence of the matrix elements of H^{sys} on the magnetic flux and the phases. Instead, we simply write $\varepsilon_{l,l'}$ and $V_{l,l'}(t)$. We shall recover the more complete notation in section VI, where we shall analyze symmetry properties that depend on those parameters. In order to simplify the notation we also adopt energy units with $\hbar = 1$.

The contacts between the system and the reservoirs are described by hopping terms of the form

$$H^{cont} = -\sum_\alpha w_\alpha (c_{k_\alpha}^\dagger c_{j_\alpha} + H.c.), \tag{21}$$

where k_α and j_α are, respectively, coordinates of the reservoirs and the central system. We assume models of free electrons for the reservoirs,

$$H^{res} = \sum_{\alpha k_\alpha} \varepsilon_{k_\alpha} c_{k_\alpha}^\dagger c_{k_\alpha}. \tag{22}$$

We also consider the possibility of applying ac-external voltages at the reservoirs, which are represented by potentials of the form (10). This introduces a time-dependent shift in the energies $\varepsilon_{k_\alpha} \to \varepsilon_\alpha(t) = \varepsilon_{k_\alpha} + eV_\alpha \cos(\Omega_0 t + \varphi_\alpha)$. Alternatively, it is possible to get rid of these time-dependent shifts by recourse to a gauge transformation $c_{k_\alpha} \to \overline{c}_{k_\alpha}(t) = c_{k_\alpha} e^{-i\int_{t_0}^{t} dt_1 eV_\alpha \cos(\Omega_0 t_1 + \varphi_\alpha)}$. Within such a procedure, the hopping matrix element of (21) becomes modified to $w_\alpha \to w_\alpha e^{-i\int_{t_0}^{t} dt_1 eV_\alpha \cos(\Omega_0 t_1 + \varphi_\alpha)}$. Both ways of tackling the problem end in the same results for the evaluated mean values of observables. We choose the first one.

The elementary theoretical tools of Keldysh formalism are the retarded, lesser, advanced, and bigger Green's functions. The first ones are defined as follows

$$G_{l,l'}^R(t,t') = \Theta(t-t')\Big[G_{l,l'}^>(t,t') - G_{l,l'}^<(t,t')\Big], \tag{23a}$$

$$G_{l,l'}^<(t,t') = i\langle c_{l'}^\dagger(t') c_l(t)\rangle, \tag{23b}$$

while the remaining functions are defined from the relations: $G_{l,l'}^>(t,t') = [G_{l',l}^<(t',t)]^*$ and $G_{l,l'}^A(t,t') = [G_{l',l}^R(t',t)]^*$. These Green's functions are used in the calculation of mean values of observables, in particular, the currents flowing through the different pieces of the driven system. Their evaluation needs the solution of the equations governing their time-evolution, which are derived from a matricial Dyson equation[42]. If we focus on spatial coordinates lying on the lattice of the central system it is convenient to define the matrices $\hat{H}^{sys}(t)$ and $\hat{G}^{R,<}(t,t')$, which have matrix elements $H_{l,l'}^{sys}(t)$ and $G_{l,l'}^{R,<}(t,t')$, respectively. The corresponding matrices for the advanced and the bigger Green's functions are obtained from the relations $\hat{G}^A(t,t') = [\hat{G}^R(t',t)]^\dagger$ and

$\hat{G}^>(t,t') = [\hat{G}^<(t',t)]^\dagger$. The Dyson equations for these Green's functions are:

$$\begin{aligned}
&\Big\{ i\overrightarrow{\frac{\partial}{\partial t}} - \hat{H}^{sys}(t)\Big\}\hat{G}^R(t,t') \\
&- \textstyle\int_{t'}^{t} dt_1 \hat{\Sigma}^R(t,t_1)\hat{G}^R(t_1,t') = \hat{1}\delta(t-t'), \\
&\hat{G}^R(t,t')\Big\{ -i\overleftarrow{\frac{\partial}{\partial t'}} - \hat{H}^{sys}(t')\Big\} \\
&- \textstyle\int_{t'}^{t} dt_1 \hat{G}^R(t,t_1)\hat{\Sigma}^R(t_1,t') = \hat{1}\delta(t-t'),
\end{aligned} \tag{24a}$$

$$\begin{aligned}
&\Big\{ i\overrightarrow{\frac{\partial}{\partial t}} - \hat{H}^{sys}(t)\Big\}\hat{G}^<(t,t') - \textstyle\int_{-\infty}^{t} dt_1 \hat{\Sigma}^R(t,t_1)\hat{G}^<(t_1,t') \\
&- \textstyle\int_{-\infty}^{t'} dt_1 \hat{\Sigma}^<(t,t_1)\hat{G}^A(t_1,t') = \hat{0}, \\
&\hat{G}^<(t,t')\Big\{ -i\overleftarrow{\frac{\partial}{\partial t'}} - \hat{H}^{sys}(t')\Big\} - \textstyle\int_{-\infty}^{t} dt_1 \hat{G}^R(t,t_1)\hat{\Sigma}^<(t_1,t') \\
&- \textstyle\int_{-\infty}^{t'} dt_1 \hat{G}^<(t,t_1)\hat{\Sigma}^A(t_1,t') = \hat{0},
\end{aligned} \tag{24b}$$

where $\overrightarrow{\partial}$ and $\overleftarrow{\partial}$ indicates that the operator acts to the right and to the left, respectively. The Dyson equations for the Green's functions with spatial coordinates outside the central region have a similar structure, considering the corresponding pieces of the Hamiltonian H instead of $\hat{H}^{sys}(t)$ and $\hat{\Sigma}^{R,>}(t,t') = 0$. In the absence of many-body interactions, the self-energies entering (24a) and (24b) take into account only the effect of the "escape to the leads". They are obtained from the Dyson equations for Green's functions with coordinates along the connections to the leads and integrating out the degrees of freedom related to the reservoirs.[20,21] Explicitly, they read:

$$\Sigma^{\lessgtr}_{l,l'}(t,t') = \delta_{l,j_\alpha}\delta_{l',j_\alpha}|w_\alpha|^2 g^{\lessgtr}_\alpha(t,t'), \tag{25}$$

and

$$\Sigma^R_{l,l'}(t,t') = \Theta(t-t')\Big[\Sigma^>_{l,l'}(t,t') - \Sigma^<_{l,l'}(t,t')\Big], \tag{26}$$

with

$$\begin{aligned}
g^{\lessgtr}_\alpha(t,t') = \pm i \sum_{k,m} e^{-ik\Omega_0 t} J_m(\frac{V_\alpha}{\Omega_0}) J_{m+k}(\frac{V_\alpha}{\Omega_0}) e^{-ik\varphi_\alpha} \\
\times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \lambda^{\lessgtr}_\alpha(\omega - m\Omega_0)\rho_\alpha(\omega - m\Omega_0),
\end{aligned} \tag{27}$$

where the density of states $\rho_\alpha(\omega) = \sum_{k_\alpha}\delta(\omega - \varepsilon_{k_\alpha})$, corresponds to H^{res}, while $\lambda^<_\alpha(\omega) = f_\alpha(\omega)$ and $\lambda^>_\alpha(\omega) = 1 - f_\alpha(\omega)$, being $f_\alpha(\omega) = 1/(e^{\beta_\alpha(\omega-\mu^0_\alpha)}+1)$, the Fermi function corresponding to the reservoir α, which is assumed to be at the temperature $1/\beta_\alpha$. This function is only well defined for equilibrium problems and is thus related only to the stationary component of the Hamiltonian H^{res}.[21] We also define the functions

$$\begin{aligned}
\Gamma_\alpha(k,\omega) &= |w_\alpha|^2 e^{-ik\varphi_\alpha} \sum_{m=-\infty}^{\infty} J_m(\frac{V_\alpha}{\Omega_0}) J_{m+k}(\frac{V_\alpha}{\Omega_0}) \\
&\quad \times \Gamma^0_\alpha(\omega - m\Omega_0), \\
\Gamma^{\lessgtr}_\alpha(k,\omega) &= |w_\alpha|^2 e^{-ik\varphi_\alpha} \sum_{m=-\infty}^{\infty} J_m(\frac{V_\alpha}{\Omega_0}) J_{m+k}(\frac{V_\alpha}{\Omega_0}) \\
&\quad \times \lambda^{\lessgtr}_\alpha(\omega - m\Omega_0)\Gamma^0_\alpha(\omega - m\Omega_0), \\
\Gamma^0_\alpha(\omega) &= |w_\alpha|^2 \rho_\alpha(\omega).
\end{aligned} \tag{28}$$

In the practical solution of the problem, the strategy followed in Ref. 28,29 was to work with convenient integral representations of the Dyson equations (24a) and (24b):

$$\begin{aligned}
&\hat{G}^R(t,t') = \hat{G}^0(t-t') + \\
&\sum_{k=-\infty}^{\infty}{}' \int_{t'}^{t} dt_1 e^{-ik\Omega_0 t_1} \hat{G}^R(t,t_1)\hat{V}(k)\hat{G}^0(t_1-t') + \\
&\sum_{k=-\infty}^{\infty}{}' \int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \frac{d\omega}{2\pi} e^{-ik\Omega_0 t_1} e^{-i\omega(t_1-t_2)} \\
&\times \hat{G}^R(t,t_1)\hat{\Sigma}(k,\omega)\hat{G}^0(t_1-t'),
\end{aligned} \tag{29a}$$

$$\begin{aligned}
\hat{G}^{\lessgtr}(t,t') = \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t'} dt_2 \hat{G}^R(t,t_1)\hat{\Sigma}^{\lessgtr}(t_1,t_2) \\
\times \hat{G}^A(t_2,t'),
\end{aligned} \tag{29b}$$

where $\sum_k{}'$ denotes $\sum_{k\neq 0}$. For the coordinates (j_α, k_α) along the contact, it is convenient to work with

$$G^R_{j_\alpha,\alpha}(t,t') = -w_\alpha \textstyle\int_{-\infty}^{t} dt_1 G^R_{j_\alpha,j_\alpha}(t,t_1) g^R_\alpha(t_1,t'), \tag{30a}$$

$$\begin{aligned}
&G^<_{j_\alpha,\alpha}(t,t') = -w_\alpha\Big\{ \textstyle\int_{-\infty}^{t} dt_1 G^R_{j_\alpha,j_\alpha}(t,t_1) g^<_\alpha(t_1,t') \\
&+ \textstyle\int_{-\infty}^{t'} dt_1 G^<_{j_\alpha,j_\alpha}(t,t_1) g^A_\alpha(t_1,t')\Big\},
\end{aligned} \tag{30b}$$

where we have defined $G^{R,<}_{j_\alpha,\alpha}(t,t') = \sum_{k_\alpha} G^{R,<}_{j_\alpha,k_\alpha}(t,t')$, while $g^R_\alpha(t,t') = \Theta(t-t')[g^>_\alpha(t,t') - g^<_\alpha(t,t')]$ and $g^A_\alpha(t,t') = [g^R_\alpha(t',t)]^*$. In equations (29a) and (29b), we have also defined:

$$\hat{\Sigma}(k,\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\hat{\Gamma}(k,\omega')}{\omega - \omega' + i0^+}, \tag{31}$$

where $\hat{\Gamma}(k,\omega)$ has matrix elements $\Gamma_{l,l'}(k,\omega) = \delta_{l,j_\alpha}\delta_{l',j_\alpha}\Gamma_\alpha(k,\omega)$. The retarded Green's function $\hat{G}^0(t-t')$ corresponds to the equilibrium problem defined by the static piece of $H^{sys}(t)$ (with matrix elements $\varepsilon_{l,l'}$) dressed by the static component of the self-energy. In other words, it is the solution of

$$[\omega\hat{1} - \hat{\varepsilon} - \hat{\Sigma}(0,\omega)]\hat{G}^0(\omega) = \hat{1}, \tag{32}$$

being

$$\hat{G}^0(\omega) = \int_{-\infty}^{t} dt' \hat{G}^0(t-t') e^{i(\omega+i0^+)(t-t')}, \qquad (33)$$

Notice that in the equation for the lesser (bigger) Green's function, we have dropped a term that depends on the solution of the homogeneous equation, which is only relevant in the description of transient behavior.

According to Refs. 28,29, we introduce the following Fourier transform for the retarded Green's function:

$$\hat{G}^R(t,\omega) = \int_{-\infty}^{t} dt' \hat{G}^R(t,t') e^{i(\omega+i0^+)(t-t')}. \qquad (34)$$

Transforming (29a) according to (34) results in the following set of linear equations

$$\hat{G}^R(t,\omega) = \hat{G}^0(\omega) + \sum_{k=-\infty}^{\infty}{}' e^{-ik\Omega_0 t} \hat{G}^R(t,\omega+k\Omega_0)\hat{V}(k)\hat{G}^0(\omega) + \sum_{k=-\infty}^{\infty}{}' e^{-ik\Omega_0 t} \hat{G}^R(t,\omega+k\Omega_0)\hat{\Sigma}(k,\omega)\hat{G}^0(\omega). \qquad (35)$$

Since the above equation is periodic in t with period $\tau_0 = \Omega_0/2\pi$, it is possible to expand its solution in Fourier series:

$$\hat{G}^R(t,\omega) = \sum_{k=-\infty}^{\infty} e^{-ik\Omega_0 t} \hat{\mathcal{G}}(k,\omega). \qquad (36)$$

Note that the above procedure takes care of causality. In fact, the transformation (34), defined with respect to the difference of the two times is the natural extension to the transformation (33) for retarded Green's functions defined in text books for stationary problems, which ensures correct analytical properties of the transformed function. In addition, notice that (36) is a Fourier series, not a Fourier transformation, which reflects the fact that Dyson equation is periodic in the "observational time" t and so does the corresponding solution. The retarded Green's function can be calculated from the solution of the linear set (35). A convenient method for the direct evaluation of the Fourier components (36) is the renormalization method of Ref. 30.

B. Current through the leads

The mean value of observables related to one-body operators can be directly expressed in terms of the lesser (or bigger) Green's function. In particular, the charge current flowing through the lead from the central system towards the reservoir α, can be written (in units of $e/\hbar$) as:

$$\begin{aligned} J_\alpha(t) &= i w_\alpha \sum_{k_\alpha} \langle c^\dagger_{k_\alpha} c_{j_\alpha} - c^\dagger_{j_\alpha} c_{k_\alpha} \rangle \\ &= 2 w_\alpha \mathrm{Re}\Big[G^<_{j_\alpha,\alpha}(t,t) \Big]. \end{aligned} \qquad (37)$$

Notice that the above current is related to the current (1) through: $I_\alpha(t) = eJ_\alpha(t)/\hbar$. Taking into account the Dyson equation describing the contact between the central system and the lead (30b) this current can be written as:

$$J_\alpha(t) = -2|w_\alpha|^2 \mathrm{Re}\Big\{ \int_{-\infty}^{t} dt_1 \Big[G^R_{j_\alpha,j_\alpha}(t,t_1) g^<_\alpha(t_1,t) + G^<_{j_\alpha,j_\alpha}(t,t_1) g^A_\alpha(t_1,t) \Big] \Big\}. \qquad (38)$$

Making use of the definition (23a), we can also express (38) as follows:

$$J_\alpha(t) = -2|w_\alpha|^2 \mathrm{Re}\Big\{ \int_{-\infty}^{t} dt_1 \Big[G^>_{j_\alpha,j_\alpha}(t,t_1) - G^<_{j_\alpha,j_\alpha}(t,t_1) \Big] g^<_\alpha(t_1,t) + G^>_{j_\alpha,j_\alpha}(t,t_1) g^A_\alpha(t_1,t) \Big\}, \qquad (39)$$

which, for the case of stationary reservoirs, simplifies to:

$$J_\alpha(t) = 2\mathrm{Im}\Big\{ \int_{-\infty}^{t} dt_1 \int_{-\infty}^{+\infty} \tfrac{d\omega}{2\pi} e^{i\omega(t-t_1)} \Gamma^0_\alpha(\omega) \times \Big[G^>_{j_\alpha,j_\alpha}(t,t_1) f_\alpha(\omega) + G^<_{j_\alpha,j_\alpha}(t,t_1) \Big(1 - f_\alpha(\omega)\Big) \Big] \Big\}. \qquad (40)$$

The above expression has an appealing form, since it depends on Boltzmann-like factors. In fact, $\Gamma^0_\alpha(\omega) f_\alpha(\omega) G^>_{j_\alpha,j_\alpha}(t,t_1)$ is related to the probability for a state in the lead α to be occupied times the probability for its closest site at the central structure, j_α, to be unoccupied, while the term $(1 - f_\alpha(\omega))\Gamma^0_\alpha(\omega) G^<_{j_\alpha,j_\alpha}(t,t_1)$ is related to the probability of the opposite process to take place.

In what follows, we focus in the dc-component of the current, which is defined as:

$$J^{dc}_\alpha = \frac{1}{\tau_0} \int_0^{\tau_0} dt J_\alpha(t). \qquad (41)$$

1. *Review of the stationary case*

Let us first consider $V_{l,l'}(t) = V_\alpha(t) = 0$ and we review the procedure introduced by Caroli et al.[43] Since in the stationary regime the Green's functions entering eq. (38) depend only on the difference of times, it is possible to perform the usual Fourier transform in the variable $t - t'$. The result is:

$$J_\alpha = -2|w_\alpha|^2 \mathrm{Re}\Big\{ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Big[G^R_{j_\alpha,j_\alpha}(\omega) g^<_\alpha(\omega) + G^<_{j_\alpha,j_\alpha}(\omega) g^A_\alpha(\omega) \Big] \Big\}. \qquad (42)$$

Then, using the following identities and definitions:

$$\begin{aligned} g^R_\alpha(\omega) &= [g^A_\alpha(\omega)]^* = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\rho_\alpha(\omega')}{\omega - \omega' + i0^+}, \\ g^<_\alpha(\omega) &= i f_\alpha(\omega) \rho_\alpha(\omega), \end{aligned} \qquad (43)$$

as well as the Dyson equation:

$$G^{<}_{j_\alpha j_\alpha}(\omega) = \sum_{\beta=1}^{N_r} G^R_{j_\alpha,j_\beta}(\omega)\Sigma^{<}_{j_\beta}(\omega)G^A_{j_\beta,j_\alpha}(\omega), \quad (44)$$

Eq. (42) can be written as:

$$J_\alpha = |w_\alpha|^2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Big\{ f_\alpha(\omega)\rho_\alpha(\omega) 2\mathrm{Im}\Big[G^R_{j_\alpha,j_\alpha}(\omega)\Big] + \sum_\beta f_\beta(\omega)\Gamma^0_\beta(\omega)|G^R_{j_\alpha,j_\beta}(\omega)|^2\Big\}. \quad (45)$$

Let us note that in the present case $\hat{G}^R(\omega) \equiv \hat{G}^0(\omega)$ with $\hat{\Sigma}(0,\omega) \equiv \hat{\Sigma}^0(\omega)$, being

$$\Sigma^0_{l,l'}(\omega) = \sum_{\alpha=1}^{N_r} \delta_{l,j_\alpha}\delta_{l',j_\alpha} \int \frac{d\omega'}{2\pi} \frac{\Gamma^0_\alpha(\omega')}{\omega - \omega' + i0^+}. \quad (46)$$

Being an equilibrium Green's function, $\hat{G}^0(\omega)$ satisfies the following property (see appendix A for a proof):

$$\mathrm{Im}\Big[G^0_{j_\alpha,j_\alpha}(\omega)\Big] = \sum_{\beta=1}^{N_r} G^0_{j_\alpha,j_\beta}(\omega)\Gamma^0_\beta(\omega)G^0_{j_\alpha,j_\beta}(\omega)^*. \quad (47)$$

Using it in (45) and recalling the definition of the self-energy (27), we get the well known expression for the current[43]:

$$J_\alpha = \sum_{\beta=1}^{N_r} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega)|G^0_{j_\alpha,j_\beta}(\omega)|^2 \Big[f_\beta(\omega) - f_\alpha(\omega)\Big]. \quad (48)$$

2. *Time-periodic local potentials with stationary reservoirs.*

Let us now consider the possibility of time-dependent terms in the Hamiltonian of the central system, but stationary reservoirs, i.e $V_\alpha(t) = 0$.

Using (29b) as well as the Fourier representation (36) in Eq. (38) we get the following expression for the dc-component of the current through the lead α:

$$J^{dc}_\alpha = \int_{-\infty}^{\infty} \tfrac{d\omega}{2\pi} \Big\{ 2\mathrm{Im}\Big[\mathcal{G}_{j_\alpha,j_\alpha}(0,\omega)\Big]\Gamma^0_\alpha(\omega)f_\alpha(\omega) + \sum_{\beta=1}^{N_r}\sum_{k=-\infty}^{\infty} |\mathcal{G}_{j_\alpha,j_\beta}(k,\omega)|^2 f_\beta(\omega)\Gamma^0_\beta(\omega)\Gamma^0_\alpha(\omega+k\Omega_0)\Big\}. \quad (49)$$

There are two additional equivalent expressions to the above dc-current, which correspond to two different representations of the term $\mathrm{Im}\Big[\mathcal{G}_{j_\alpha,j_\alpha}(0,\omega)\Big]$. The first one is obtained from the condition of the continuity of the current, as shown in appendix B. An alternative proof is given in appendix C. Substituting (B2) in (49) results in the following representation:

$$J^{dc}_\alpha = \sum_{\beta\neq\alpha=1}^{N_r}\sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \times \Big\{ |\mathcal{G}_{j_\alpha,j_\beta}(k,\omega)|^2 \Gamma^0_\beta(\omega)\Gamma^0_\alpha(\omega+k\Omega_0)f_\beta(\omega) - |\mathcal{G}_{j_\beta,j_\alpha}(k,\omega)|^2 \Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega+k\Omega_0)f_\alpha(\omega)\Big\}. \quad (50)$$

The second additional representation corresponds to substituting the identity (D4) derived in appendix D into (49). The result is:

$$J^{dc}_\alpha = \sum_{\beta=1}^{N_r}\sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Gamma^0_\beta(\omega)\Gamma^0_\alpha(\omega+k\Omega_0) \times |\mathcal{G}_{j_\alpha,j_\beta}(k,\omega)|^2 \Big[f_\beta(\omega) - f_\alpha(\omega+k\Omega_0)\Big]. \quad (51)$$

Any of the three representations (49), (50) and (51) are equally valid to calculate the dc-current flowing through the lead α. The concrete evaluation implies the solution of the retarded Green's function from the Dyson equation (35) with $\hat{\Sigma}(k,\omega) = 0$.

3. *Time-dependent voltages at the reservoirs.*

Let us finally consider the more general case, where, in addition to the pumping potentials at the central structure, ac voltages are applied at the reservoirs.

We start from the definition of the time-dependent current through lead α (39) and substitute there Eqs. (27) and (29b). Then, we use the Fourier representation of the retarded Green's function (36) and take the dc-component. The result is:

$$J^{dc}_\alpha = \sum_{\beta=1}^{N_r}\sum_{k,q,p=-\infty}^{\infty} \mathrm{Re}\Big\{ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \times [\Gamma_\alpha(p,\omega+k\Omega_0)\Gamma^{<}_\beta(q,\omega) - \Gamma^{<}_\alpha(p,\omega+k\Omega_0)\Gamma_\beta(q,\omega)] \times \mathcal{G}_{j_\alpha,j_\beta}(k-q+p,\omega+q\Omega_0)\mathcal{G}^*_{j_\alpha,j_\beta}(k,\omega)\Big\}. \quad (52)$$

Equivalently, this expression can also be written as:

$$J^{dc}_\alpha = \sum_{\beta=1}^{N_r}\sum_{k,q,p=-\infty}^{\infty} J_{n+p}(\frac{eV_\alpha}{\Omega_0})J_n(\frac{eV_\alpha}{\Omega_0}) \times J_{m+q}(\frac{eV_\beta}{\Omega_0})J_m(\frac{eV_\beta}{\Omega_0})\mathrm{Re}\Big\{ e^{i(p\varphi_\alpha+q\varphi_\beta)} \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Gamma^0_\alpha(\omega) \times \Gamma^0_\beta(\omega+(n-k-m)\Omega_0)\Big[f_\beta(\omega+(n-k-m)\Omega_0) - f_\alpha(\omega)\Big]\mathcal{G}_{j_\alpha,j_\beta}(k-q+p,\omega+(n-k+q)\Omega_0) \times \mathcal{G}^*_{j_\alpha,j_\beta}(k,\omega+(n-k)\Omega_0)\Big\}. \quad (53)$$

For reservoirs with a smooth density of states such that $\Gamma^0_\alpha(\omega - m\Omega_0) \sim \Gamma_\alpha(\omega)$ and $\Gamma^0_\beta(\omega - m\Omega_0) \sim \Gamma_\beta(\omega)$, the expression for the dc-current further simplifies. In fact, in such a case (52) reduces to:

$$J_\alpha^{dc} = \sum_{\beta=1}^{N_r} \sum_{k,q,m=-\infty}^{\infty} \mathrm{Re}\Big\{ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Gamma_\alpha^0(\omega)\Gamma_\beta^0(\omega) \Big[e^{iq\varphi_\beta} \times$$
$$f_\beta(\omega - m\Omega_0) J_{m+q}(\frac{eV_\beta}{\Omega_0}) J_m(\frac{eV_\beta}{\Omega_0}) \mathcal{G}_{j_\alpha,j_\beta}(k-q,\omega+q\Omega_0)$$
$$\mathcal{G}^*_{j_\alpha,j_\beta}(k,\omega) - e^{iq\varphi_\alpha} f_\alpha(\omega + (k-m)\Omega_0) J_{m+q}(\frac{eV_\alpha}{\Omega_0})$$
$$\times J_m(\frac{eV_\alpha}{\Omega_0}) \mathcal{G}_{j_\alpha,j_\beta}(k+q,\omega)\mathcal{G}^*_{j_\alpha,j_\beta}(k,\omega) \Big] \Big\}, \tag{54}$$

where we have used the first summation formula for products of Bessel functions given in appendix E. Performing a shift $\omega \to \omega - k\Omega_0$ in the second term of (54) and making use of the identity (D4), it is also possible to recast the above expression as:

$$J_\alpha^{dc} = \sum_{qm=-\infty}^{\infty} \mathrm{Re}\Big\{ \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Big[\Gamma_\alpha^0(\omega) \times$$
$$\sum_{\beta=1}^{N_r} \sum_{k=-\infty}^{\infty} \Big(e^{iq\varphi_\beta} J_{m+q}(\frac{eV_\beta}{\Omega_0}) J_m(\frac{eV_\beta}{\Omega_0}) \Gamma_\beta^0(\omega) \times$$
$$\mathcal{G}_{j_\alpha,j_\beta}(k-q,\omega+q\Omega_0)\mathcal{G}^*_{j_\alpha,j_\beta}(k,\omega) f_\beta(\omega - m\Omega_0) \Big)$$
$$-ie^{iq\varphi_\alpha} J_{m+q}(\frac{eV_\alpha}{\Omega_0}) J_m(\frac{eV_\alpha}{\Omega_0}) \Big(\mathcal{G}_{j_\alpha j_\alpha}(q,\omega)$$
$$-\mathcal{G}^*_{j_\alpha,j_\alpha}(-q,\omega+q\Omega_0) \Big) f_\alpha(\omega - m\Omega_0) \Big] \Big\}. \tag{55}$$

In summary, expressions (52) and (53) define two equivalent ways to calculate the dc current through the lead α in the case of ac voltages at reservoirs with arbitrary densities of states, while (54) and (55) are two equivalent representations of such current for reservoirs with smooth densities of states.

In any of these cases, the evaluation of J_α^{dc} implies the solution of the complete set (35).

IV. TRANSLATION BETWEEN THE TWO FORMALISMS

We propose the following translation between the Floquet S-matrix and the Green's functions:

$$S_{F,\alpha\beta}(E_m,E_n) = \delta_{\alpha,\beta}\delta_{m-n,0} - \tag{56}$$
$$i\sqrt{\Gamma_\alpha^0(\omega+m\Omega_0)\Gamma_\beta^0(\omega+n\Omega_0)}\mathcal{G}_{j_\alpha,j_\beta}(m-n,\omega+n\Omega_0),$$

with $E_m = \omega + m\Omega_0$.

It is important to note that this translation exactly recovers all the representations for the dc current derived in the framework of Floquet scattering matrix theory in the case of stationary reservoirs. In fact, translating (50) and (51) according to (57), leads to equations (8) and (9), respectively. In addition, in eq. (50) it is possible to identify the transfer matrix formulation of Refs. 31 and 32:

$$T_{\alpha\beta}(E,E_k) = |\mathcal{G}_{j_\alpha,j_\beta}(k,\omega)|^2 \Gamma_\beta^0(\omega)\Gamma_\alpha^0(\omega+k\Omega_0), \tag{57}$$

being $\alpha \neq \beta$.

For stationary problems, we should consider $m = n = 0$ and $\mathcal{G}_{j_\alpha j_\beta}(k,\omega) \to G^0_{j_\alpha,j_\beta}(\omega)$ in (57), in which case, we recover an expression like the one proposed in Ref. 35:

$$S^0_{\alpha\beta}(E) = \delta_{\alpha,\beta} -$$
$$i\sqrt{\Gamma_\alpha^0(\omega)\Gamma_\beta^0(\omega)} G^0_{j_\alpha,j_\beta}(\omega), \tag{58}$$

In the case of reservoirs with ac-voltages described by wide-band models with smooth densities of states, such that $\Gamma_\alpha(\omega \pm k\Omega_0) \sim \Gamma_\alpha(\omega)$, the translation (57) also transforms Eq.(55) into Eq.(13).

V. PROOF OF THE UNITARY PROPERTY OF $\hat{S}_F$.

In the S-matrix formalism, current conservation implies that the scattering matrix is unitary, see Eqs.(4). In what follows we show that, for static reservoirs, this property can be proved by using identities satisfied by the Green's functions as well as the translation formula (57). In fact, let us use Eq.(57) inside the summations of the left hand side of Eq. (4b):

$$\sum_{\beta=1}^{N_r} \sum_{n=-\infty}^{\infty} S^*_{F,\alpha\beta}(E,E_n) S_{F,\gamma\beta}(E_m,E_n) =$$
$$\delta_{\alpha\gamma}\delta_{m,0} - \sqrt{\Gamma_\gamma^0(\omega+m\Omega_0)\Gamma_\alpha^0(\omega)} \Big[i\mathcal{G}_{j_\gamma,j_\alpha}(m,\omega) -$$
$$i\mathcal{G}^*_{j_\alpha,j_\gamma}(-m,\omega+m\Omega_0) - \sum_{\beta=1}^{N_r}\sum_{n=-\infty}^{\infty} \mathcal{G}_{j_\gamma,j_\beta}(m-n,\omega+n\Omega_0)$$
$$\times \Gamma_\beta^0(\omega+n\Omega_0)\mathcal{G}^*_{j_\alpha,j_\beta}(-n,\omega+n\Omega_0) \Big]. \tag{59}$$

From the identity (D3), it can be shown that the second term of the right hand side of the above equation vanishes identically, thus recovering equation (4b).

Similarly, using Eq.(57) inside the summations of the left hand side of Eq. (4a):

$$\sum_{\alpha=1}^{N_r} \sum_{n=-\infty}^{\infty} S^*_{F,\alpha\beta}(E_n,E) S_{F,\alpha\gamma}(E_n,E_m) =$$
$$\delta_{\beta\gamma}\delta_{m,0} + \sqrt{\Gamma_\gamma^0(\omega+m\Omega_0)\Gamma_\beta^0(\omega)} \Big[i\mathcal{G}^*_{j_\gamma,j_\beta}(m,\omega) -$$
$$i\mathcal{G}_{j_\beta,j_\gamma}(-m,\omega+m\Omega_0) + \sum_{\alpha=1}^{N_r}\sum_{n=-\infty}^{\infty} \mathcal{G}^*_{j_\alpha,j_\beta}(n,\omega)$$
$$\times \Gamma_\alpha^0(\omega+n\Omega_0)\mathcal{G}_{j_\alpha,j_\gamma}(-m+n,\omega+m\Omega_0) \Big], \tag{60}$$

and from the identity (C6), equation (4a) is recovered.

The same procedure can be followed to prove the unitarity of the S-matrix in the case of reservoirs with oscillating voltages at the reservoirs, provided the density of states of the reservoirs is smooth.

VI. ADIABATIC APPROXIMATION WITHIN KELDYSH FORMALISM.

A. Definition

The adiabatic point of view is inspired in a parametrical representation of the time dependent terms of the Hamiltonian. This means a description where the observation time t is assumed to be frozen in the equations governing the dynamics of the system. In particular, instead of the Dyson equation (35), in a frozen description we must consider the following equation

$$\hat{G}^f(t,\omega) = \hat{G}^0(\omega) + \sum_{k=-\infty}^{\infty}{}' e^{-ik\Omega_0 t}\hat{G}^f(t,\omega)\hat{V}(k)\hat{G}^0(\omega) + \sum_{k=-\infty}^{\infty}{}' e^{-ik\Omega_0 t}\hat{G}^f(t,\omega)\hat{\Sigma}(k,\omega)\hat{G}^0(\omega) \quad (61)$$

which is a stationary Dyson equation corresponding to the strength of the parameters $\hat{V}(t)$ and $V_\alpha(t)$ at the observation time t. As the potentials are periodic in t, the frozen Green's function can be expanded in a Fourier series:

$$\hat{G}^f(t,\omega) = \sum_{k=-\infty}^{\infty} e^{-ik\Omega_0 t}\hat{\mathcal{G}}^f(k,\omega), \quad (62)$$

and through the translation (58) it is possible to define the Fourier coefficients $\hat{S}_0(k,E) \equiv \hat{S}_{0,k}(E)$ for the elements of the frozen S-matrix as

$$S_{0,\alpha\beta}(k,E) = \delta_{\alpha,\beta}\delta_{k,0} - i\sqrt{\Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega)}\mathcal{G}^f_{j_\alpha,j_\beta}(k,\omega). \quad (63)$$

In the Floquet S-matrix formalism, the adiabatic approximation is given by Eqs.(15). In analogy to Eq.(15a) we propose the following ansatz for the $\propto \Omega_0$ approximation to the Green's function:

$$\hat{\mathcal{G}}^R(k,\omega) \sim \hat{\mathcal{G}}^f(k,\omega) + \frac{k\Omega_0}{2}\frac{\partial\hat{\mathcal{G}}^f(k,\omega)}{\partial\omega} + \Omega_0\hat{a}(k,\omega), \quad (64)$$

or, equivalently,

$$\hat{G}(t,\omega) \sim \hat{G}^f(t,\omega) + i\frac{1}{2}\frac{\partial^2\hat{G}^f(t,\omega)}{\partial t\partial\omega} + \Omega_0\hat{a}(t,\omega), \quad (65)$$

where $\hat{\mathcal{G}}^f(k,\omega)$ (or $\hat{G}^f(t,\omega)$) is the *frozen* Green's function, which obeys the equilibrium Dyson equation (61). The substitution of the ansatz Eq.(64) with the translation formula (57) into Eq.(15a) leads to the following relation between $A_{\alpha\beta}$ and a_{j_α,j_β}:

$$A_{\alpha\beta}(k,E) = -i\sqrt{\Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega)}a_{j_\alpha,j_\beta}(k,\omega) - i\frac{k\Omega_0}{4}\sqrt{\Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega)}\mathcal{G}^f_{j_\alpha,j_\beta}(k,\omega) \Big[\frac{1}{\Gamma^0_\alpha(\omega)}\frac{\partial\Gamma^0_\alpha(\omega)}{\partial\omega} - \frac{1}{\Gamma^0_\beta(\omega)}\frac{\partial\Gamma^0_\beta(\omega)}{\partial\omega}\Big],$$
$$A_{\alpha\beta}(t,E) = -i\sqrt{\Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega)}a_{j_\alpha,j_\beta}(t,\omega) + \frac{1}{4}\sqrt{\Gamma^0_\alpha(\omega)\Gamma^0_\beta(\omega)}\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)}{\partial t} \Big[\frac{1}{\Gamma^0_\alpha(\omega)}\frac{\partial\Gamma^0_\alpha(\omega)}{\partial\omega} - \frac{1}{\Gamma^0_\beta(\omega)}\frac{\partial\Gamma^0_\beta(\omega)}{\partial\omega}\Big]. \quad (66)$$

In Ref. 17, some important properties of the matrix $\hat{A}$ have been proved on the basis of the unitary property of $\hat{S}_F$ and the fact that for a Hamiltonian of spinless fermions that depends on a magnetic flux Φ and on time-dependent potentials of the form

$$V_{l,l'}(t) = \delta_{l,l'}\sum_j \delta_{l,j}[V^0_j + V^1_j\cos(\omega t + \delta_j)], \quad (67)$$

the stationary matrix transforms under $t \to -t$ as:

$$S_{0,\alpha\beta}(k,E,\Phi,\delta) = S_{0,\alpha\beta}(-k,E,\Phi,-\delta), \quad (68)$$

as well as

$$S_{0,\alpha\beta}(k,E,-\Phi,\delta) = S_{0,\beta\alpha}(k,E,\Phi,\delta). \quad (69)$$

Analogously, the Hamiltonian is invariant under the simultaneous change of $t \to -t$ and $\delta_j \to -\delta_j$. Therefore,

$$\mathcal{G}^f_{l,l'}(k,\Phi,\delta_j,\omega) = \mathcal{G}^f_{l,l'}(-k,\Phi,-\delta_j,\omega). \quad (70)$$

In addition, in the presence of a magnetic flux Φ, the static terms of the Hamiltonian of the system satisfy $\varepsilon_{l,l'}(\Phi) = \varepsilon_{l',l}(-\Phi) = [\varepsilon_{l',l}(\Phi)]^*$, which implies:

$$G^f_{l,l'}(t,\Phi,\omega) = G^f_{l',l}(t,-\Phi,\omega). \quad (71)$$

In other words, the frozen Green's function $\mathcal{G}^f_{j_\alpha,j_\beta}(k,\omega)$ has the same symmetry properties of $S_{0,\alpha\beta}(k,\omega)$. Therefore, from Eq. (66) we see that $a_{j_\alpha j_\beta}$ has the same symmetry properties as $A_{\alpha\beta}$.

In order to calculate $\hat{a}(k,\omega)$ explicitly, we have to consider the Dyson equation for the Fourier coefficients of the retarded Green's function, which can be obtained by expanding (35) in Fourier series:

$$\hat{\mathcal{G}}(k,\omega) = \hat{G}^0(\omega)\delta_{k,0} + \sum_{k'=-\infty}^{\infty}{}' \hat{\mathcal{G}}(k+k',\omega+k'\Omega_0)\hat{V}(k')\hat{G}^0(\omega) + \sum_{k'=-\infty}^{\infty}{}' \hat{\mathcal{G}}(k+k',\omega+k'\Omega_0)\hat{\Sigma}(k',\omega)\hat{G}^0(\omega), \quad (72)$$

then substitute (64) and keep terms up to the first order in Ω_0. The solution of the ensuing linear set allows for the evaluation of $\hat{a}(k,\omega)$ as a function of the stationary Green functions $\hat{G}^0(\omega)$, the frozen Green functions $\hat{\mathcal{G}}^f(k,\omega)$ and the derivatives $\partial\hat{\mathcal{G}}^f(k,\omega)/\partial\omega$ and $\partial\hat{G}^0(\omega)/\partial\omega$. Alternatively, in order to get $\hat{a}(t,\omega)$, we have to substitute the ansatz (65) in the Dyson equation (35), keep terms up to $\propto\Omega_0$ and solve the resulting linear set, which gives $\hat{a}(t,\omega)$ as a function of $\hat{G}^f(t,\omega)$, $\partial^2\hat{G}^f(t,\omega)/\partial t\partial\omega$, $\hat{G}^0(\omega)$, and $\partial\hat{G}^0(\omega)/\partial\omega$.

B. Calculation of the dc current

1. Time-periodic local potentials with stationary reservoirs

In order to calculate the adiabatic approximation to the dc-current through the leads in the case of stationary reservoirs it is convenient to start from Eq. (51). Expanding that expression in powers of Ω_0 and keeping up to the linear term, the dc-current reads:

$$J_\alpha^{dc} \sim \frac{1}{\tau_0}\int_0^{\tau_0} dt \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Big[\frac{\partial f_\alpha(\omega)}{\partial\omega}J_\alpha^{(pump)}(t,\omega) + \Big(f_\beta(\omega)-f_\alpha(\omega)\Big)\Big(J_\alpha^{(bias)}(t,\omega)+J_\alpha^{(int)}(t,\omega)\Big)\Big], \quad (73)$$

being

$$J_\alpha^{(pump)}(t,\omega) = \Gamma_\alpha^0(\omega)\Gamma_\beta^0(\omega)\times \sum_{\beta=1}^{N_r}\frac{1}{2}\Big[iG^f_{j_\alpha,j_\beta}(t,\omega)\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)^*}{\partial t}+c.c.\Big], \quad (74a)$$

$$J_\alpha^{(bias)}(t,\omega) = \sum_{\beta=1}^{N_r}|G^f_{j_\alpha,j_\beta}(t,\omega)|^2\Gamma_\alpha^0(\omega)\Gamma_\beta^0(\omega), \quad (74b)$$

$$J_\alpha^{(int)}(t,\omega) = \sum_{\beta=1}^{N_r}\frac{1}{2}\frac{\partial\Gamma_\alpha^0(\omega)}{\partial\omega}\Gamma_\beta^0(\omega)\times \Big[-iG^f_{j_\alpha,j_\beta}(t,\omega)\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)^*}{\partial t}+c.c.\Big] + \frac{\Gamma_\alpha^0(\omega)\Gamma_\beta^0(\omega)}{2}\Big[-i\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)}{\partial\omega}\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)^*}{\partial t} + \Omega_0\Big(G^f_{j_\alpha,j_\beta}(t,\omega)a_{j_\alpha,j_\beta}(t,\omega)+c.c.\Big)\Big], \quad (74c)$$

For the case of reservoirs with identical chemical potentials and temperatures, such that $f_\alpha(\omega)=f_0(\omega),\forall\alpha$, only the pumping term (74a) contributes. This term is $\propto\Omega_0$ and can be shown to be equivalent to Eq.(18b) through the translation formula (57). The second term is the usual stationary contribution (48). The "interference" term ($\propto\Omega_0(\mu_\beta-\mu_\alpha)$) is a small contribution in the limit of small static bias $\mu_\beta-\mu_\alpha$. However, it may give rise to interesting behavior in the presence of magnetic field. In particular, in a two terminal set-up it is an odd function of a magnetic field [17], in striking contrast with a stationary conductance which is an even function of a magnetic field.

2. Time-dependent voltages at the reservoirs.

In order to derive the $\propto\Omega_0$ contribution to the dc current, we substitute the adiabatic approximation to the Green's function (64) in (52) and we expand the remaining terms up to $\mathcal{O}(\Omega_0^2)$. The latter step results in the following expansion:

$$\Gamma_\alpha(p,\omega+k\Omega_0)\Gamma_\beta^<(q,\omega)-\Gamma_\alpha^<(p,\omega+k\Omega_0)\Gamma_\beta(q,\omega) \sim \sum_{m,n-\infty}^{\infty}J_{n+p}(\frac{eV_\alpha}{\Omega_0})J_n(\frac{eV_\alpha}{\Omega_0})J_{m+q}(\frac{eV_\beta}{\Omega_0})J_m(\frac{eV_\beta}{\Omega_0}) \times e^{i(p\varphi_\alpha+q\varphi_\beta)}\Big\{\Gamma_\alpha(\omega)\Gamma_\beta(\omega)\Big[f_\beta(\omega)-f_\alpha(\omega)\Big] + \Omega_0\Big[(k-n)g_1(\omega)-mg_2(\omega)\Big]+\Omega_0^2\Big[g_3(\omega)(k-n)^2 + m^2g_4(\omega)+m(n-k)g_5(\omega)\Big]\Big\}, \quad (75)$$

being

$$\begin{aligned}
g_1(\omega) &= \Gamma_\beta(\omega)\Big\{\frac{\partial\Gamma_\alpha(\omega)}{\partial\omega}\Big[f_\beta(\omega)-f_\alpha(\omega)\Big] -\Gamma_\alpha(\omega)\frac{\partial f_\alpha(\omega)}{\partial\omega}\Big\},\\
g_2(\omega) &= \Gamma_\alpha(\omega)\Big\{\frac{\partial\Gamma_\beta(\omega)}{\partial\omega}\Big[f_\beta(\omega)-f_\alpha(\omega)\Big] +\Gamma_\beta(\omega)\frac{\partial f_\beta(\omega)}{\partial\omega}\Big\},\\
g_3(\omega) &= \frac{\Gamma_\beta(\omega)}{2}\Big\{\frac{\partial^2\Gamma_\alpha(\omega)}{\partial\omega^2}\Big[f_\beta(\omega)-f_\alpha(\omega)\Big] -\Gamma_\alpha(\omega)\frac{\partial^2 f_\alpha(\omega)}{\partial\omega^2}\Big\},\\
g_4(\omega) &= \frac{\Gamma_\alpha(\omega)}{2}\Big\{\frac{\partial^2\Gamma_\beta(\omega)}{\partial\omega^2}\Big[f_\beta(\omega)-f_\alpha(\omega)\Big] +\Gamma_\beta(\omega)\frac{\partial^2 f_\beta(\omega)}{\partial\omega^2}\Big\},\\
g_5(\omega) &= \frac{\partial\Gamma_\alpha(\omega)}{\partial\omega}\frac{\partial\Gamma_\beta(\omega)}{\partial\omega}\Big[f_\beta(\omega)-f_\alpha(\omega)\Big]. \quad (76)
\end{aligned}$$

When substituting in (52) we use the properties of the Bessel function enunciated in appendix E and keep only terms proportional to Ω_0 and V_α. The resulting expression shows a rather compact form in the case of reservoirs with smooth densities of states and the same chemical potentials and temperature, such that $f_\alpha(\omega)=f_0(\omega),\forall\alpha$, in which case $g_5(\omega)=0$, while $g_1(\omega)=-g_2(\omega)$ and $g_3(\omega)=-g_4(\omega)$. Terms $\propto\partial^2 f_0(\omega)/\partial\omega^2$ can be reduced to terms $\propto\partial f_0(\omega)/\partial\omega$ by integrating by parts. The final result can be written by collecting the different terms in three kinds of contributions as in Eq.(18):

$$J_\alpha^{dc} \sim \frac{1}{\tau_0}\int_0^{\tau_0} dt \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\frac{\partial f_0(\omega)}{\partial \omega} \times \Big[J_\alpha^{(pump)}(t,\omega) + J_\alpha^{(rect)}(t,\omega) + J_\alpha^{(int)}(t,\omega)\Big], \quad (77)$$

with $J_\alpha^{(pump)}(t,\omega)$ given by (74a) and

$$J_\alpha^{(rect)}(t,\omega) = \sum_{\beta=1}^{N_r} G^f_{j_\alpha,j_\beta}(t,\omega) G^f_{j_\alpha,j_\beta}(t,\omega)^* \times \Gamma_\alpha(\omega)\Gamma_\beta(\omega)\Big[V_\alpha(t) - V_\beta(t)\Big], \quad (78a)$$

$$J_\alpha^{(int)}(t,\omega) = \sum_{\beta=1}^{N_r} \Gamma_\alpha(\omega)\Gamma_\beta(\omega) \times V_\beta(t)\Big\{\frac{1}{2}\Big[i\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)}{\partial\omega}\frac{\partial G^f_{j_\alpha,j_\beta}(t,\omega)^*}{\partial t} + c.c\Big] + 2\Omega_0\Big[G^f_{j_\alpha,j_\beta}(t,\omega) a_{j_\alpha,j_\beta}(t,\omega)^* + c.c.\Big]\Big\}. \quad (78b)$$

Through the translation formula (57), we can identify the three terms (74a), (78a) and (78b) with (18b), (18c) and (18d), obtained with the S-matrix formalism. In the derivation of the expression for the interference term (78b) we have made use of (D4) expressed in the adiabatic approximation (64) and an equivalent equation satisfied by the frozen Green function:

$$\mathcal{G}^f_{j_\alpha,j_\alpha}(k,\omega) - \mathcal{G}^f_{j_\alpha,j_\alpha}(k,\omega)^* = -i\sum_{k'\beta}\mathcal{G}^f_{j_\alpha,j_\beta}(k+k',\omega)\Gamma^0_\beta(\omega)\mathcal{G}^f_{j_\alpha,j_\beta}(k',\omega)^*, \quad (79)$$

which leads to the following relation:

$$\frac{k}{2}\sum_{\beta=1}^{N_r}\sum_{k'=-\infty}^{\infty}\Gamma^0_\beta(\omega)\mathcal{G}^f_{j_\alpha,j_\beta}(k+k',\omega)\frac{\partial \mathcal{G}^f_{j_\alpha,j_\beta}(k',\omega)^*}{\partial\omega} = \sum_{\beta=1}^{N_r}\sum_{k'=-\infty}^{\infty}\Gamma^0_\beta(\omega)\Big\{\mathcal{G}^f_{j_\alpha,j_\beta}(k+k',\omega)a_{j_\alpha,j_\beta}(k',\omega)^* + a_{j_\alpha,j_\beta}(k+k',\omega)\mathcal{G}^f_{j_\alpha,j_\beta}(k',\omega)^* - \frac{k'}{2}\Big[\mathcal{G}^f_{j_\alpha,j_\beta}(k+k',\omega)\frac{\partial\mathcal{G}^f_{j_\alpha,j_\beta}(k',\omega)^*}{\partial\omega} + \frac{\partial\mathcal{G}^f_{j_\alpha,j_\beta}(k+k',\omega)}{\partial\omega}\mathcal{G}^f_{j_\alpha,j_\beta}(k',\omega)^*\Big]\Big\}. \quad (80)$$

VII. SUMMARY AND CONCLUSIONS

Starting from the formulation of Keldysh non-equilibrium approach to systems in the presence of time-periodic fields of Ref. 29, we have shown several identities satisfied the Green's function. This has allowed us for the derivation of several useful equations to calculate the current (in particular, the dc-component of the current) flowing between the reservoirs and the mesoscopic system. We have considered two different situations: (i) Driving induced by voltages applied at the central structure. (ii) Driving induced by voltages applied at the reservoirs. In both cases we have considered reservoirs with a general density of states. We have also proposed an expression that enables the translation between Green's function formalism and the Floquet Scattering matrix formalism of Refs. 15,16,17. In the case (i), we have shown that this formula is able to translate exactly the expressions for the dc current flowing through the leads obtained in the two formalisms. Furthermore, we have shown that it is enough to derive the unitary property of the scattering matrix by recourse to properties of the Green's functions. In the situation (ii) we were also able to translate expressions for the current and to demonstrate the unitary property of S_F if we assume within the Green's function formalism models of reservoirs with a smooth density of states.

We have also formulated the so called adiabatic approximation to the dc-current in the framework of the non-equilibrium Green's function formalism. We have used it to derive the different contributions to the dc-current linear in the driving frequency in the two situations (i) and (ii) described above. Making use of the translation formula of section IV, it is possible to compare these expressions with the ones previously derived in the framework of Scattering matrix theory[15,16,17]. The equivalence is complete in the cases of stationary reservoirs as well as in the case of oscillating reservoirs with a smooth density of states.

VIII. ACKNOWLEDGMENTS

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APPENDIX A:

In the stationary system with $V_{l,l'}(t) = V_\alpha(t) = 0$, the Dyson equation for the retarded Green function is simply

Eq. (32). From there, we can write

$$
\begin{aligned}
&\hat{G}^0(\omega) - \hat{G}^0(\omega)^\dagger = \\
= \;& \Big\{\hat{1}\omega - \hat{\varepsilon} - \hat{\Sigma}^0(\omega)\Big\}^{-1} - \Big\{\hat{1}\omega - \hat{\varepsilon}^\dagger - \hat{\Sigma}^0(\omega)^\dagger\Big\}^{-1} \\
= \;& \Big\{\hat{1}\omega - \hat{\varepsilon} - \hat{\Sigma}^0(\omega)\Big\}^{-1} \\
&\times\Big\{\hat{1}\omega - \hat{\varepsilon}^\dagger - \hat{\Sigma}^0(\omega)^\dagger\Big\}\Big\{\hat{1}\omega - \hat{\varepsilon}^\dagger - \hat{\Sigma}^0(\omega)^\dagger\Big\}^{-1} \\
- \;& \Big\{\hat{1}\omega - \hat{\varepsilon} - \hat{\Sigma}^0(\omega)\Big\}^{-1}\Big\{\hat{1}\omega - \hat{\varepsilon} - \hat{\Sigma}^0(\omega)\Big\} \\
&\times\Big\{\hat{1}\omega - \hat{\varepsilon}^\dagger - \hat{\Sigma}^0(\omega)^\dagger\Big\}^{-1} \\
= \;& \hat{G}^0(\omega)\Big\{\hat{\Sigma}^0(\omega) - \hat{\Sigma}^0(\omega)^\dagger\Big\}\hat{G}^0(\omega)^\dagger, \qquad \text{(A1)}
\end{aligned}
$$

where we have used the fact that $\hat{\varepsilon} = \hat{\varepsilon}^\dagger$.

APPENDIX B:

Let us start from the definition of the dc current flowing through the lead α, Eq.(49). The condition of the continuity of the current implies:

$$
\begin{aligned}
&\sum_{\alpha=1}^{N_r} J_\alpha^{dc} = 0 \\
&= 2\sum_{\alpha=1}^{N_r}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathrm{Im}\Big[\mathcal{G}_{j_\alpha,j_\alpha}(0,\omega)\Big]f_\alpha(\omega) + \sum_{\alpha=1}^{N_r}\sum_{k=-\infty}^{\infty} \\
&\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}f_\beta(\omega)|\mathcal{G}_{j_\alpha,j_\beta}(k,\omega)|^2\Gamma^0_\beta(\omega)\Gamma^0_\alpha(\omega+k\Omega_0). \qquad \text{(B1)}
\end{aligned}
$$

Since the above equation must hold for arbitrary chemical potentials and temperatures of the reservoirs, the terms multiplying the Fermi functions $f_\alpha(\omega)$ have to vanish for each α, which means:

$$
-2\mathrm{Im}\Big[\mathcal{G}_{j_\alpha,j_\alpha}(0,\omega)\Big] = \sum_{\beta=1}^{N_r}\sum_{k=-\infty}^{\infty}|\mathcal{G}_{j_\beta,j_\alpha}(k,\omega)|^2\Gamma^0_\beta(\omega+k\Omega_0). \qquad \text{(B2)}
$$

APPENDIX C:

We present the proof of an important identity for the retarded Green's function. This identity has been previously proved for the case of static reservoirs in Ref. 32 within the framework of a different formalism.

We first perform a Fourier transform in $t-t'$ in the first equation of the set (24a) and take the adjoint in the spacial indices of that equation. The result is:

$$
\begin{aligned}
&\Big\{i\frac{\overrightarrow{\partial}}{\partial t} + (\omega' + i0^+) - \hat{H}^{sys}(t)\Big\}\hat{G}^R(t,\omega') \\
&-\int_{-\infty}^{t} dt_1 e^{i\omega'(t-t_1)}\hat{\Sigma}^R(t,t_1)\hat{G}(t_1,\omega') = \hat{1}, \qquad \text{(C1)} \\
&\hat{G}^R(t,\omega)^\dagger\Big\{-i\frac{\overleftarrow{\partial}}{\partial t} + (\omega - i0^+) - \hat{H}^{sys}(t)\Big\} \\
&-\int_{-\infty}^{t} dt_1 e^{-i\omega(t-t_1)}\hat{G}^R(t_1,\omega)^\dagger\hat{\Sigma}^R(t,t_1)^\dagger = \hat{1}. \qquad \text{(C2)}
\end{aligned}
$$

Note that, unlike the stationary case, these equations are not simplified to a linear set of equations and the inverse of the Green's function must be represented in terms of integro-differential operators. By multiplying (C1) from the left by $\hat{G}^R(t,\omega)^\dagger$ and (C2) from the right by $\hat{G}^R(t,\omega')$ and then subtracting the two resulting equations we get

$$
\begin{aligned}
&\hat{G}^R(t,\omega)^\dagger - \hat{G}^R(t,\omega') = i\frac{\partial}{\partial t}\Big[\hat{G}^R(t,\omega)^\dagger\hat{G}^R(t,\omega')\Big] + \\
&(\omega'-\omega)\hat{G}^R(t,\omega)^\dagger\hat{G}^R(t,\omega') - \\
&\int_{-\infty}^{t} dt_1 e^{i\omega'(t-t_1)}\hat{G}^R(t,\omega)^\dagger\hat{\Sigma}^R(t,t_1)\hat{G}^R(t_1,\omega') + \\
&\int_{-\infty}^{t} dt_1 e^{-i\omega(t-t_1)}\hat{G}^R(t_1,\omega)^\dagger\hat{\Sigma}^R(t,t_1)^\dagger\hat{G}^R(t,\omega'). \qquad \text{(C3)}
\end{aligned}
$$

If we now perform the expansions in Fourier series for $\hat{G}^R(t,\omega)$ and $\hat{G}^R(t,\omega')^\dagger$, we obtain:

$$
\begin{aligned}
&\hat{\mathcal{G}}(-k,\omega)^\dagger - \hat{\mathcal{G}}(k,\omega') = \\
&(\omega'-\omega+k\Omega_0)\sum_{k'=-\infty}^{\infty}\hat{\mathcal{G}}(k',\omega)^\dagger\hat{\mathcal{G}}(k+k',\omega') - \\
&\sum_{k',k''=-\infty}^{\infty}\hat{\mathcal{G}}^\dagger(k',\omega)\Big\{\hat{\Sigma}(k'',\omega'+(k+k'-k'')\Omega_0) - \\
&\hat{\Sigma}(k'',\omega+k'\Omega_0)^\dagger\Big\}\hat{\mathcal{G}}(k+k'-k'',\omega'). \qquad \text{(C4)}
\end{aligned}
$$

For $\omega' = \omega - k\Omega_0$, the above equation reduces to

$$
\begin{aligned}
&\hat{\mathcal{G}}(-k,\omega)^\dagger - \hat{\mathcal{G}}(k,\omega-k\Omega_0) = \\
&\sum_{k',k''}\hat{\mathcal{G}}(k',\omega)^\dagger\Big\{\hat{\Sigma}^\dagger(k'',\omega+(k'-k'')\Omega_0) - \\
&\hat{\Sigma}(k'',\omega+k'\Omega_0)\Big\}\hat{\mathcal{G}}(k+k'-k'',\omega-k\Omega_0). \qquad \text{(C5)}
\end{aligned}
$$

In the case of stationary reservoirs, the above equation further reduces to

$$
\begin{aligned}
&\hat{\mathcal{G}}(-k,\omega)^\dagger - \hat{\mathcal{G}}(k,\omega-k\Omega_0) = \\
&\sum_{k'=-\infty}^{\infty}\hat{\mathcal{G}}(k',\omega)^\dagger\Big[\hat{\Sigma}^0(\omega+k'\Omega_0)^\dagger - \\
&\hat{\Sigma}^0(\omega+k'\Omega_0)\Big]\hat{\mathcal{G}}(k+k',\omega-k\Omega_0), \qquad \text{(C6)}
\end{aligned}
$$

which, for $k=0$, reads:

$$\hat{\mathcal{G}}(0,\omega)-\hat{\mathcal{G}}(0,\omega)^{\dagger}=\sum_{k=-\infty}^{\infty}\hat{\mathcal{G}}(k,\omega)^{\dagger}\Big[\hat{\Sigma}^{0}(\omega+k\Omega_0)-\hat{\Sigma}^{0}(\omega+k\Omega_0)^{\dagger}\Big]\hat{\mathcal{G}}(k,\omega). \tag{C7}$$

Note that the identity (B2) derived in the previous appendix is a particular case of this equation.

The above identities are also valid in the case of oscillating reservoirs with smooth densities of states, as can be verified by using the fact that $\Gamma^0_\alpha(\omega+k\Omega_0)\sim\Gamma^0_\alpha(\omega)$ in (31) as well as the first of the summation formulas of products of Bessel functions of appendix E.

APPENDIX D:

In this appendix we prove another important identity satisfied by the Green's function. We start from the definitions (23a) and (23b) of the different Green's functions in Keldysh formalism and use Dyson equations for the lesser and bigger components (29b), as well as the Fourier representation of the retarded Green's function. We get:

$$\hat{G}^R(t,t')=-i\Theta(t-t')\sum_{\alpha=1}^{N_r}\sum_{k_1k_2k_3-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\hat{\Gamma}(k_2,\omega)\times e^{-i[\omega(t-t')+\Omega_0(k_1t-k_3t')]}\hat{\mathcal{G}}(k_1,\omega+k_2\Omega_0)\hat{\mathcal{G}}(k_3,\omega)^{\dagger}. \tag{D1}$$

Transforming the above Green's function according to (34) and (36) allows us to write the following spectral representation:

$$\hat{\mathcal{G}}(k,\omega)=\sum_{k'k''=-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\times\frac{\hat{\mathcal{G}}(k+k',\omega'+k''\Omega_0)\hat{\Gamma}(k'',\omega')\hat{\mathcal{G}}(k',\omega')^{\dagger}}{\omega-(\omega'+k'\Omega_0)+i0^+}. \tag{D2}$$

For the case of stationary reservoirs, it is easy to prove from the above expression the following identity:

$$\hat{\mathcal{G}}(k,\omega)-\hat{\mathcal{G}}(-k,\omega+k\Omega_0)^{\dagger}=-i\sum_{k'=-\infty}^{\infty}\hat{\mathcal{G}}(k+k',\omega-k'\Omega_0)\times\hat{\Gamma}^0(\omega-k'\Omega_0)\hat{\mathcal{G}}(k',\omega-k'\Omega_0)^{\dagger}, \tag{D3}$$

which for $k=0$ reduces to:

$$\hat{\mathcal{G}}(0,\omega)-\hat{\mathcal{G}}(0,\omega)^{\dagger}=-i\sum_{k'=-\infty}^{\infty}\hat{\mathcal{G}}(k',\omega-k'\Omega_0)\times\hat{\Gamma}^0(\omega-k'\Omega_0)\hat{\mathcal{G}}(k',\omega-k'\Omega_0)^{\dagger}. \tag{D4}$$

The above identities are also valid in the case of reservoirs with oscillating voltages provided that they are described by a wide-band model with a smooth density of states such that $\Gamma^0_\alpha(\omega-m\Omega_0)\sim\Gamma^0_\alpha(\omega)$. This can be easily proved by using the first of the summation formulae of appendix E.

APPENDIX E:

Products of Bessel functions satisfy the following summation formulas:

$$\sum_{n=-\infty}^{\infty}J_{n+p}(X)J_n(X)=\delta_{p,0},$$
$$\sum_{n=-\infty}^{\infty}J_{n+p}(X)J_n(X)n=X(\delta_{p,1}+\delta_{p,-1})$$
$$\sum_{n=-\infty}^{\infty}J_{n+p}(X)J_n(X)n^2=\frac{X^2}{2}\delta_{p,0}-X\Big[(p-\frac{1}{2})\delta_{p,1}-(p+\frac{1}{2})\delta_{p,-1}\Big]+\frac{X^2}{4}(\delta_{p,2}+\delta_{p,-2}). \tag{E1}$$

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