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Transport properties of a mesoscopic metallic loop connected to leads

L. Arrachea[a]

Scuola Internazionale Superiore di Studi Avanzati (SISSA) and Istituto Nazionale per la Fisica della Materia (INFM) (Unitá di Ricerca Trieste-SISSA), Via Beirut n. 4, 34013 Trieste, Italy

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Abstract. We study the transport properties of a metallic ring threaded by a magnetic flux varying linearly in time $\Phi_M(t) = \Phi t$ with a constriction and connected to two external particle reservoirs. This setup contains as limiting cases the experimental arrangements used to define Kubo and Landauer conductances. We employ a formalism based in Baym-Kadanoff-Keldysh non-equilibrium Green functions to calculate the conductance of the system and the dissipated power. We compare the transport behavior in different limits of the geometrical configuration.

PACS. 72.10.Bg General formulation of transport theory – 73.40.Jn Metal-to-metal contacts – 73.40.Gk Tunneling

1 Introduction

Landauer and Büttiker formalism to study electron transport in 1D mesoscopic systems has been one of the most successful theoretical ideas of condensed matter physics [1,2]. In this description, a voltage V is applied to the system under study by connecting it to two external reservoirs at different chemical potentials μ_α and $\mu_\beta = \mu_\alpha + eV$. An scheme of the typical setup is depicted in Figure 1a. The concept of electron conduction is related with the transmission properties of the sample as a response to the voltage V. In particular, at zero temperature, the current flowing through the sample is expressed as

$$J_L = \frac{2e}{\hbar} \int_{\mu_\alpha}^{\mu_\beta} d\omega T(\omega), \qquad (1)$$

where $T(\omega)$ is the transmission function. It is remarkable that J_L remains finite even for ideal noninteracting systems. The fact that a "perfect conductor" has a finite resistance caused consternation in the community some time ago and an important amount of work has been devoted to understand this issue [3,4]. In the first derivation, Landauer formula was slightly different from (1) and the conductance was proportional to the quotient between transmission and reflection coefficients [1]. It was later clarified that such a definition corresponds to the ratio between the current flowing through the device and the potential drop between the ends of the wire. The latter differs from the applied voltage V by an amount corresponding to the potential drop due to the "contact" resistance

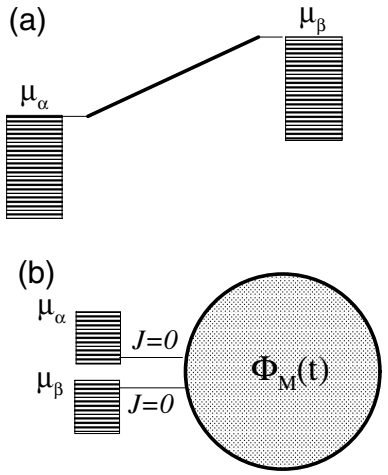

Fig. 1. (a) Scheme of the typical device considered to define Landauer conductance. The ends of the wire under study are connected to two reservoirs with chemical potentials μ_α and μ_β. (b) Scheme of a device to define Kubo conductance. The wire is closed at its ends to form a ring which is threaded by a time-dependent magnetic flux. Inelastic scattering events are introduced by coupling it to reservoirs through passive leads that do not transport any current.

[a] *Permanent address*: Departamento de Física, Universidad de Buenos Aires, Ciudad Universitaria Pabellón I, (1428) Buenos Aires, Argentina
e-mail: arrachea@mpipks-dresden.mpg.de

[2,3]. The existence of such a resistance can be understood by noting that the external reservoirs, besides establishing a potential difference between the ends of the system, introduce resistive behavior and energy dissipation. In an ideal situation, an electron can propagate coherently along the system. However, as soon as it travels through the connecting lead and visits the particle reservoir, it experiments inelastic scattering processes and losses its phase coherence. This means that the function $T(\omega)$ does not really measure the conducting properties of the sample we want to investigate, but those of a combined system which consists of our sample in interaction with the reservoirs.

An alternative framework to study the transport properties of a quantum system is that leading to the celebrated Kubo formula for the electric conductivity. In this approach the concept of conduction is related to the response of the system to an external electric field [5]. Most of the derivations and conclusions related to the appropriate way to define the conductance of a quantum wire connected to leads at different potentials, were achieved by recourse to linear response theory starting from an electric field applied on the mesoscopic sample [4,6–9]. In spite of the many subtleties related to the coupling to the semi-infinite leads and the boundary conditions for the external field, the main goal of those works has been to establish the equivalence of Landauer and Kubo formulations for geometrical setups like that of Figure 1a, suitably generalized to support additional channels and terminals in some cases.

In the same spirit of Kubo approach, Büttiker, Imry and Landauer [10] considered a 1D system closed at its ends to form a ring and examined a situation where it is pierced by a time-dependent magnetic flux. In this case, a current is established, driven by the induced electric field. For a linearly increasing magnetic flux $\Phi_M(t) = \Phi t$ and when the sample is an ideal noninteracting metal isolated from the external world, it is found to display Bloch oscillations with a vanishing mean value of the current and a period depending on the magnitude of the induced electric field $E = (1/cL)d\Phi_M(t)/dt$ and the length of the circumference L. This feature is a consequence of the coherent nature of the charge propagation along the system and in this sense, it could be interpreted as the time-dependent counterpart of the Aharanov-Bohm oscillations observed in mesoscopic rings threaded by static magnetic fluxes [11]. An important conceptual difference between both kinds of quantum oscillations is that in the time-dependent problem, Bloch oscillations are related with quanta of stored energy that can be dissipated when the ring is put in contact with another system. In the most general case, the interaction with the external world introduces inelastic scattering processes in our wire and phase coherence is broken when the carrier propagates beyond a typical length. In addition, energy dissipation is associated with the existence of a dc-component in the current flowing along the system. The idea that some resistance is necessary to obtain a net nonvanishing current in this device is in contrast with our intuition since it is natural to relate a "perfect conductor" with that capable of transporting current with zero resistance. This important conceptual point has been analyzed in the pioneer work by Landauer and Büttiker [12] and has been further elaborated during the subsequent years [13–15].

Therefore, when a dissipative mechanism is included as an ingredient of the annular driven system, a conductance can be defined as the response of the dc-current as a function of the induced emf $(e/c)d\Phi_M(t)/dt$. A concrete way to introduce inelastic scattering events is to couple the ring to external reservoirs. This idea was first proposed by Büttiker to investigate the transport properties of a mesoscopic metal loop threaded by a magnetic flux with an harmonic dependence on time [16] and was later considered in several other studies [17,18,21]. The idea of bending the wire into a ring threaded by a time-dependent magnetic flux, as a basic device to calculate the conductance as define by Kubo, has been recently employed in non-interacting metallic systems with barriers [19,20]. In the present work, we shall seek a geometry close to the device of Figure 1a, considering the ring coupled to particle reservoirs through passive leads that allow inelastic scattering without transporting current as indicated in Figure 1b. Although the contact with only one reservoir is enough in order to introduce inelastic scattering events in the problem [16,21], two reservoirs must be consider in order to define an experimental arrangement with the same "degree of inelastic scattering" of that introduced by Landauer. There are recent works where this geometry has been considered [18–20] and the issue Landauer vs. Kubo definitions has been discussed in non-interacting systems under ac-pumping and with disorder [18]. Our goal is to study a simpler case where the flux varies in time following a linear law in a system without disorder. As this problem can be solved exactly, we can investigate further details of the transport properties of this kind of devices.

In a recent paper [21] the problem of a metallic ring of non-interacting electrons threaded by a magnetic flux with a linear time-dependence and coupled to an external reservoir was studied in the framework of nonequilibrium Green functions. This formalism has been very successful to derive generalized transport equations [22,23] in quantum systems in contact with leads and reservoirs that are described by Hamiltonians with and without an explicit time dependence. One of its advantages is that the effect of leads and reservoirs can be concisely described by means of self-energies with a finite imaginary part. Thus, the associated concept of irreversibility is introduced in a very natural way and features like the finite resistance of a "perfect conductor" have a rather straightforward representation. For the case of our simple device it is possible to define a closed set of equations for the retarded Green functions in real space which is amenable to be numerically solved, yielding to the exact solution for the relevant currents flowing through the system. In this work, we adapt the treatment presented in [21] to the geometrical configuration sketched in Figure 2, which contains the two geometries of Figure 1 as limiting cases while also allows for more general configurations interpolating between them. We calculate the dc-component of the induced

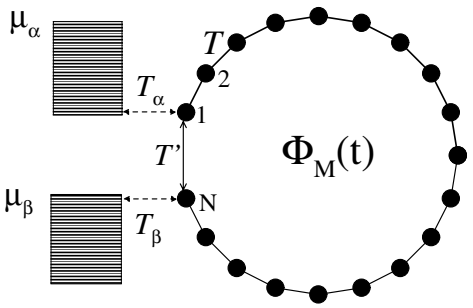

Fig. 2. Model for the general setup considered in our study. The wire is described by a chain of N noninteracting tight-binding electrons with hopping amplitude T. The contacts with the reservoirs are represented by the hopping elements T_α and T_β. The hopping element T' represents a constriction for $T' < T$.

current as a function of Φ and we compare with the predictions of Landauer scheme for an equivalent dc-voltage. We also introduce a method to calculate exactly the dissipated power and we obtain the behavior expected from the Joule effect. Although the formalism is valid for any strength of Φ, we focus on the range within the scope of linear response theory.

The paper is organized as follows: In Section 2 we introduce the model and we present the basic theoretical treatment. Results are shown in Section 3 and Section 4 is devoted to summary and conclusions.

2 Theoretical treatment

We introduce a model for the setup sketched in Figure 2. It consists on a ring with a constriction in one of the arms, which is threaded by a magnetic flux with a linear time-dependence $\Phi_M(t) = \Phi t$ and connected to reservoirs at different chemical potentials. We present the relevant equations to describe the electron transport and we derive the equations to compute the dissipated energy.

2.1 The model

We assume that the full system can be described by the following Hamiltonian:

$$H = H_{ring}(t) + H_\alpha + H_\beta + H_{1\alpha} + H_{N\beta}, \qquad (2)$$

where the first term, representing the ring, depends explicitly on time due to the presence of the time-dependent flux. We consider noninteracting spinless electrons (the spin does not play any relevant role in the physical properties we want study) described by a tight-binding model with N sites and lattice constant $a = L/N$,

$$H_{ring} = -T \sum_{l=1}^{N-1} \left(e^{-i\phi t} c_l^\dagger c_{l+1} + e^{i\phi t} c_{l+1}^\dagger c_l \right) - T' \left(e^{-i\phi t} c_1^\dagger c_N + e^{i\phi t} c_N^\dagger c_1 \right). \qquad (3)$$

The time-dependent phase ϕt attached to each link, with $\phi = \Phi/(\Phi_0 N)$, accounts for the presence of the external magnetic flux. A different hopping element T' in the bond labeled as $\langle 1, N\rangle$ represents a constriction for $T' < T$. The terms H_α and H_β describe the left and right leads in contact with particle reservoirs with chemical potentials μ_α and μ_β, respectively, while

$$H_{1\alpha} = -T_\alpha \left(c_1^\dagger c_\alpha + c_\alpha^\dagger c_1 \right),$$
$$H_{N\beta} = -T_\beta \left(c_N^\dagger c_\beta + c_\beta^\dagger c_N \right), \qquad (4)$$

represent the connections between the ring and the leads in contact to the reservoirs.

2.2 The currents

In order to calculate the current along the different parts of the circuit, we use a treatment based on non-equilibrium Green functions. We follow the same lines of reference [21] and we defer the reader to this work and references therein for further details.

In the framework of the formalism proposed by Keldysh, the perturbation expansion has the same structure as the formalism for equilibrium systems. The different feature in the non-equilibrium case is that the Green functions are contour-ordered rather than time-ordered. As a consequence, the Dyson equation has a matrix form and one must work with two independent Green functions: the retarded Green function,

$$G^R_{i,j}(t,t') = -i\Theta(t-t') \left\langle \left\{ c_i(t), c_j^\dagger(t') \right\} \right\rangle, \qquad (5)$$

and the lesser than Green function

$$G^<_{i,j}(t,t') = i \left\langle c_i^\dagger(t) c_j(t') \right\rangle. \qquad (6)$$

The latter determines the mean values of the observables. In particular, the current through a bond $\langle i,j\rangle$ is written as

$$J_{i,j} = \frac{2e}{\hbar} \mathrm{Re}\left[T_{ij} G^<_{i,j}(t,t) \right], \qquad (7)$$

where T_{ij} is the corresponding hopping element.

After some algebraic manipulation on the Dyson equation [22,23], the effect of the external leads and reservoirs can be exactly written in terms of self-energy corrections at the sites $1(N)$ of the tight-binding chain. This represents the effect of the escape to the leads in

contact with the reservoirs (systems α and β, respectively). The ensuing retarded and lesser components of these self-energies are

$$\Sigma^R_{1(N)}(t-t') = \left|T_{\alpha(\beta)}\right|^2 g^R_{\alpha(\beta)}(t-t'),$$

$$\Sigma^<_{1(N)}(t-t') = \left|T_{\alpha(\beta)}\right|^2 g^<_{\alpha(\beta)}(t-t'), \tag{8}$$

where $g^{R,<}_{\alpha(\beta)}(t-t')$ are the retarded and lesser components of the Green functions corresponding to the systems $\alpha(\beta)$, respectively. The numerical procedure to compute the currents is simplified if the electronic structure of each of these systems is assumed to be well described by a constant density of states Γ (we assume that α and β have the same band structure), and very large bandwidths. We also assume that the contacts are identical, thus $T_\alpha = T_\beta$. Within such a model, the self energies result $\Sigma^R_{1(N)}(\omega) = i\sigma$, and $\Sigma^<_{1(N)}(\omega) = if_{\alpha(\beta)}(\omega)\sigma$, being $\sigma = |T_\alpha|^2\Gamma$. The Fermi functions $f_{\alpha(\beta)}(\omega)$ depend on the chemical potentials μ_α, μ_β and temperatures of the reservoirs. For sake of simplicity, we assume that these temperatures are equal to zero. Thus, $f_\alpha(\omega) = \Theta(\omega - \hbar^{-1}\mu_\alpha)$ and $f_\beta(\omega) = \Theta(\omega - \hbar^{-1}\mu_\beta)$. A remarkable issue is that the self-energies have an imaginary part. This feature indicates that the presence of leads and reservoirs introduces dissipative effects in the problem. We recall that without this ingredient, the dc-component of the current vanishes and only Bloch oscillations take place [10,12,21].

It is convenient [21] to perform a gauge transformation in the fermionic operators of the Hamiltonian (3),

$$c_n = \exp[in\phi t]\overline{c}_n, \tag{9}$$

according to which the Green function for the positions m, n on the ring transforms as

$$G^R_{m,n}(t,t') = \exp\left[i\phi(mt - nt')\right]\overline{G}^R_{m,n}(t,t'), \tag{10}$$

while the Hamiltonian must be transformed to

$$\begin{aligned}\overline{H}_{ring} &= \overline{H_0} + \overline{H}_{1N}(t)\\ &= -T\sum_{l=1}^{N-1}\left(\overline{c}^\dagger_l\overline{c}_{l+1} + \overline{c}^\dagger_{l+1}\overline{c}_l\right) + \sum_{l=1}^{N} V_l\overline{c}^\dagger_l\overline{c}_l\\ &\quad - \left(T_{1N}(t)\overline{c}^\dagger_1\overline{c}_N + T_{N1}(t)\overline{c}^\dagger_N\overline{c}_1\right),\end{aligned} \tag{11}$$

where $T_{1N}(t) = [T_{N1}(t)]^* = T'e^{-i\Phi t}$ while $V_l = \hbar\phi l$ is the scalar potential due to the induced electric field. In this way, the explicit time-dependent part of the Hamiltonian is confined to a single bond. The currents are, of course, gauge-invariant quantities and the final expressions for the ones between the ring and the reservoirs, and that along the bond $\langle l, l+1\rangle$ of the ring, are found to be

$$\begin{aligned}J_{1,\alpha}(t) &= \frac{2e}{\hbar}\sigma\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\Bigg[f_\alpha(\omega-\phi)\Bigg(\mathrm{Im}\left[\overline{G}^R_{1,1}(t,\omega)\right]\\ &\quad + \sigma\left|\overline{G}^R_{1,1}(t,\omega)\right|^2\Bigg) + \sigma f_\beta\left(\omega - \frac{\Phi}{\Phi_0}\right)\\ &\quad \times\left|\overline{G}^R_{1,N}(t,\omega)\right|^2\Bigg],\\ J_{N,\beta}(t) &= \frac{2e}{\hbar}\sigma\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\Bigg[f_\beta\left(\omega - \frac{\Phi}{\Phi_0}\right)\Bigg(\mathrm{Im}\left[\overline{G}^R_{N,N}(t,\omega)\right]\\ &\quad + \sigma\left|\overline{G}^R_{N,N}(t,\omega)\right|^2\Bigg) + \sigma f_\alpha(\omega-\phi)\left|\overline{G}^R_{N,1}(t,\omega)\right|^2\Bigg],\\ J_{l,l+1}(t) &= \frac{2eT_{l,l+1}}{\hbar}\sigma\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\mathrm{Im}\Bigg[f_\alpha(\omega-\phi)\overline{G}^R_{l,1}(t,\omega)\\ &\quad \times\overline{G}^A_{1,l+1}(\omega,t) + f_\beta\left(\omega - \frac{\Phi}{\Phi_0}\right)\overline{G}^R_{l,N}(t,\omega)\\ &\quad \times\overline{G}^A_{N,l+1}(\omega,t)\Bigg],\end{aligned} \tag{12}$$

where $G^A_{i,j}(\omega,t) = [G^R_{j,i}(t,\omega)]^*$ is the advanced Green function, while the Fourier transform of the retarded Green function is defined as,

$$G^R_{i,j}(t,\omega) = \int_{-\infty}^{t} dt' e^{i(\omega+i\eta)(t-t')}G^R_{i,j}(t,t'), \tag{13}$$

with $\eta = 0^+$. The hopping element is $T_{l,l+1} = T$ if $l = 1,\ldots,N-1$ and $T_{l,l+1} = T'$ if $l = N$. Note that the gauge transformation introduces frequency shifts and that the *effective* chemical potentials in the expressions for the currents are $\mu^{eff}_\alpha = \mu_\alpha + \hbar\phi$ and $\mu^{eff}_\beta = \mu_\beta + \hbar\Phi/\Phi_0$. The practical calculation of the currents requires the evaluation of the retarded Green functions. A summary of the procedure is given in Appendix A.

It is useful to write the current along the ring as

$$J_{l,l+1}(t) = \frac{2eT_{l,l+1}}{\hbar}\sigma\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}T(t,\omega,\Delta), \tag{14}$$

where we define the "transmission" function as

$$\begin{aligned}T(t,\omega,\Delta) = \mathrm{Im}\Big[&(f_\alpha(\omega-\phi)\overline{G}^R_{l,1}(t,\omega)\overline{G}^A_{1,l+1}(\omega,t)\\ &+ f_\alpha(\omega-\Delta)\overline{G}^R_{l,N}(t,\omega)\overline{G}^A_{N,l+1}(\omega,t)\Big],\end{aligned} \tag{15}$$

being $\Delta = \hbar^{-1}eV + \Phi/\Phi_0$, where eV is the potential difference between the two external reservoirs, $eV = \mu_\beta - \mu_\alpha$.

We now turn to analyze some details corresponding to the different possible choices of boundary conditions imposed by the chemical potentials of the reservoirs. Let us begin examining this issue with a brief review of the

transport behavior of the metal loop threaded by a flux $\Phi(t) = \Phi t$ in contact to only one reservoir analyzed in detail in reference [21]. When the ring is connected to *only one* lead, all the currents, i.e. that along the loop and that between the loop and the reservoir, display an oscillating behavior as functions of time with the period $\tau = 2\pi\Phi/\Phi_0$. The latter effect is due to the Bloch oscillations in the system, which are driven by the induced constant electric field and which result as a consequence of the coherent propagation of the carriers along the loop. The connection to the lead and reservoir introduces inelastic scattering events which attenuates the amplitude of the oscillations while introduces a dc-component in the current along the ring. The dc-component of the current between ring and reservoir is, however, always zero, irrespective the strengths of the inelastic scattering, the electric field and the chemical potential of the reservoir. The lead, thus plays a passive role, in the sense that neither pumps nor sucks a net amount of charge in the loop. The dc-current and the conductance of the device so defined correspond to Kubo picture, since the only driving force is the induced electric field. In the case of the *two terminals* considered here, caution must be taken in defining conditions that represent passive leads. In fact, an arbitrary choice for the difference $\mu_\beta - \mu_\alpha = eV$, generates, in general, a non-vanishing dc-component of the currents $J^{dc}_{N,\beta}$ and $J^{dc}_{1,\alpha}$. To define Kubo conductance in this geometry and to constraint the leads to play a passive role, we fix eV in order to satisfy $J^{dc}_{N,\beta} = J^{dc}_{1,\alpha} = 0$, which implies that the net charge transport along the ring is driven by the electric field alone. The calculation of V satisfying this constraint is accomplished in the numerical solution of the problem. The integrals (12) are evaluated numerically. As explained in Appendix A, the retarded Green function is obtained from the solution of set (27). We define the Kubo current as the dc-component of the current flowing along the ring under the above mentioned conditions,

$$J_K = \frac{1}{\tau}\int_0^\tau dt J_{l,l+1}(t). \tag{16}$$

Note that since the leads do not transport any dc-current, J_K does not depend on the particular bond considered for the calculation of $J_{l,l+1}(t)$.

The geometry to define Landauer conductance corresponds to a problem which is independent of time. We start from the general time-dependent formulation, we perform the gauge transformation (9) and consider afterward the operation of cutting the loop. The latter is achieved by taking the limit $T' \to 0$ at the constriction. In addition, the chemical potentials are considered as boundary conditions that match the drop V_l of the scalar potential. Thus, the difference is fixed to satisfy $\mu_\beta - \mu_\alpha = \hbar\Phi/\Phi_0$. The latter condition allows for a net charge current to flow from one of the reservoirs to the other traveling along the chain. This compensates the otherwise interruption due to the cut of the circuit imposed by the vanishing hopping element at the constriction. In Appendix B it is shown that the resulting expression for J_L is

$$J_L = \frac{2e}{\hbar}\sigma^2 \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left[f_\beta(\omega) - f_\alpha(\omega)\right] \left|G^0_{1,N}(\omega)\right|^2, \tag{17}$$

where $G^0_{1,N}(\omega)$ is the Green function of the problem defined by the "unperturbed" part $\overline{H}_0$ of the Hamiltonian (11) ($\overline{H}$ with $T' = 0$). Note that in the limit $T' = 0$, where the loop is cut, the non-conservative forces that drive the movement of charge along the circuit are interrupted. Formally, this implies that the Hamiltonian describing the system does no longer depend on time and that there are no frequency shifts introduced by the transformation (10). As a consequence, the chemical potentials in the evaluation of J_L are μ_β and μ_α, i.e. directly those of the reservoirs. Instead, when the loop is closed ($T' \neq 0$) the effective chemical potentials μ^{eff}_β and μ^{eff}_α take into account not only the chemical potentials of the reservoirs but also the shifts due to the presence of the induced emf. Another detail is that in the literature it is frequently found the evaluation of J_L by considering $\Phi = 0$ in the evaluation of $G^0_{1,N}(\omega)$. This procedure is valid only for very small Φ, in which case J_L can be approximated by a linear function of Φ. In this setup, the transmission function analogous to (15) reads

$$T_L(\omega, \Delta) = \left[f_\alpha(\omega - \Delta) - f_\alpha(\omega)\right] \left|G^0_{1,N}(\omega)\right|^2, \tag{18}$$

where $\Delta = \hbar^{-1}eV$.

To close this section we mention that we also consider an "interpolating" configuration between the above mentioned Landauer and Kubo geometries, which corresponds to the full time dependent problem with a finite, but small $0 < T' \leq T$ (a constriction). The chemical potential difference is fixed to satisfy the matching condition with the scalar potential drop. Taking into account the energy shifts introduced by the gauge transformation, this corresponds to $\mu^{eff}_\beta - \mu^{eff}_\alpha = \hbar\Phi/\Phi_0$, which is equivalent to consider $eV = \mu_\beta - \mu_\alpha = \hbar\phi$ in the evaluation of the "transmission" functions (15) and the currents (12). We emphasize that when the loop is closed, the effective chemical potentials in the evaluation of the currents are not the bare ones of the reservoirs, but those modified by the presence of the emf. It is, therefore, the difference between them the relevant one to define a boundary condition equivalent to that of Landauer geometry. As discussed previously, this condition allows for a net flow of charge between the reservoirs and the loop. Then, $J^{dc}_{N,\beta} = -J^{dc}_{1,\alpha} \neq 0$ and the current along the loop results as the combined effect of this flow and the movement of charge driven by the induced emf. The latter relation between the currents along the leads can be inferred from geometrical considerations.

2.3 The dissipated energy

When the coupling with external elements like leads and reservoirs is taken into account, the ring behaves as an

open system that exchanges not only electrons but also energy. This issue was analyzed by Büttiker [16] in a ring coupled to a single lead connected to a reservoir while threaded by a magnetic flux with an harmonic time-dependence. Although the physical situation in that case corresponds to a wire exposed to a microwave field and it is somewhat different from the one considered in the present work, the feature to highlight is the dissipation of energy originated in the coupling to the external system. In what follows, we explain how to calculate exactly the energy dissipated when a dc-current is flowing along our wire by using the nonequilibrium Green function formalism.

We recall that we assume that the Hamiltonian (2) describes the ring as well as the environment. The macroscopic leads behave as a thermal bath and their contact with the small system enables the absorption of energy supplied by the external field. An estimate of the rate at which the energy is transferred from the field into the bath through the metallic ring is given by the variation of the average energy E_{ring} stored in the ring per unit time,

$$P(t) = \frac{E_{ring}}{dt} = -\frac{i}{\hbar}\left\langle [H_{ring}, H] \right\rangle , \tag{19}$$

being H the full Hamiltonian (2). In terms of Green functions it can be written as,

$$P(t) = \frac{2}{\hbar}\mathrm{Re}\Big[T_\alpha (Te^{-i\phi t}G^<_{2,\alpha}(t,t) + T'e^{i\phi t}G^<_{N,\alpha}(t,t)) + T_\beta \left(Te^{i\phi t}G^<_{N-1,\beta}(t,t) + T'e^{-i\phi t}G^<_{1,\beta}(t,t)\right)\Big]. \tag{20}$$

After some algebra on the Dyson equation for the above lesser Green functions and assuming a wide-band model for the systems α and β, it is obtained

$$\begin{aligned} P(t) = \frac{2\sigma}{\hbar}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\Big\{ & f_\alpha(\omega-\phi)\Big[T\mathrm{Im}\left(\overline{G}^R_{2,1}(t,\omega)\right) \\ & + \sigma\mathrm{Re}\Big(\left(T\overline{G}^R_{2,1}(t,\omega) + T'e^{i\frac{\Phi}{\Phi_0}t}\overline{G}^R_{N,1}(t,\omega)\right) \\ & \times \overline{G}^A_{1,1}(\omega,t) + \Big(T\overline{G}^R_{N-1,1}(t,\omega) + T'e^{-i\frac{\Phi}{\Phi_0}t}\overline{G}^R_{1,1}(t,\omega)\Big) \\ & \times \overline{G}^A_{1,N}(\omega,t)\Big)\Big] + f_\beta\left(\omega-\frac{\Phi}{\Phi_0}\right)\Big[T\mathrm{Im}\left(\overline{G}^R_{N-1,N}(t,\omega)\right) \\ & + \sigma\mathrm{Re}\Big(\left(T\overline{G}^R_{N-1,N}(t,\omega) + T'e^{-i\frac{\Phi}{\Phi_0}t}\overline{G}^R_{1,N}(t,\omega)\right) \\ & \times \overline{G}^A_{N,N}(\omega,t) + \Big(T\overline{G}^R_{2,N}(t,\omega) \\ & + T'e^{i\frac{\Phi}{\Phi_0}t}\overline{G}^R_{N,N}(t,\omega)\Big)\overline{G}^A_{N,1}(\omega,t)\Big)\Big]\Big\}, \end{aligned} \tag{21}$$

which can be evaluated numerically by solving the equations for the retarded Green functions as indicated in Appendix A. This quantity is an oscillating function of time with the period τ of the Bloch oscillations. The dissipated power is given by

$$P_D = \frac{1}{\tau}\int_0^\tau dt P(t). \tag{22}$$

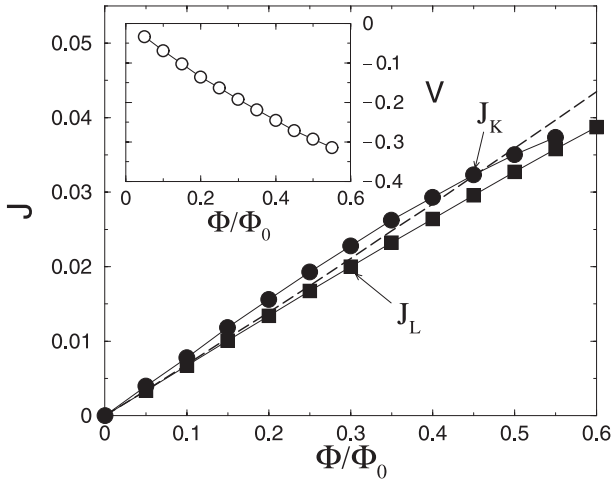

Fig. 3. Currents along the wire corresponding to Landauer (squares) and Kubo (circles) geometries as functions of the induced scalar potential $\hbar\Phi/\Phi_0$ for a chain of $N = 200$ sites with $\sigma = 0.8T$ and $\mu_\alpha = -T$. The linear approximation for J_L is indicated in dashed lines. Inset: The voltage $V = (\mu_\beta - \mu_\alpha)/e$, consistent with the condition of vanishing currents in the leads in the Kubo case.

3 Results

The behavior of the Kubo and Landauer currents J_K and J_L as functions of the voltage $\hbar\Phi/\Phi_0$ between the ends of the wire is shown in Figure 3 for a chain with $N = 200$ sites. We have also analyzed other lengths corresponding to chains with a number of sites between $N = 20$ and $N = 2000$ without finding significant quantitative changes in the dc-response. The particular value $\sigma = 0.8T$ in the self energy correction due to the escape to the leads has been assumed in the simulations. For $T' \neq 0$ the currents display an oscillating behavior as a function of t similar to that observed in the case of only one lead [21]. At each step of our calculations we verified the continuity of the dc-current by evaluating it explicitly along the different components of the circuit as a check of consistency of our approach.

For the case of the Landauer current the dashed lines indicate the result for the linear approximation corresponding to consider $\Phi = 0$ in the evaluation of $G^0_{1,N}(\omega)$. For the case of the Kubo current it is shown in the inset the chemical potential difference $\mu_\beta - \mu_\alpha = eV$ that, for each value of Φ, is consistent with the constraint of vanishing current in the leads ($J^{dc}_{1,\alpha} = J^{dc}_{N,\beta} = 0$). In this way, the current through the bond $\langle 1, N\rangle$ is the same as the current along the other arm of the ring. The external leads connected to the reservoirs play the role of dissipators and do not pump neither suck charge in the ring.

The most salient feature in the results shown in Figure 3 is the fact that J_K is larger than J_L within the range of interest $\Phi/\Phi_0 < T$. The difference between the two kind of responses is not enormous but sizable within our numerical precision. The remaining part of this section is devoted to the analysis of this discrepancy. To this end we refer to the set of equations (27) which provides the

solution for the retarded Green function. This set is obtained by performing the Fourier transform at fixed time t in the Dyson equation for the retarded Green function (cf. Eq. (13)). It can be seen that the same set is obtained by writing the Dyson equation for the retarded Green function of a problem defined by the effective "noninteracting" Hamiltonian

$$H^0_{eff} = \sum_{n,\nu} \left(E_\nu + n\hbar \frac{\Phi}{\Phi_0} \right) |\nu, n\rangle\langle\nu, n| \qquad (23)$$

and the "perturbation"

$$H'_{eff} = -T_{1N}(t)|1, n\rangle\langle N, n+1| - T_{N1}(t)|N, n+1\rangle\langle 1, n|, \qquad (24)$$

where E_ν and $|\nu\rangle$ are the eigenvalues and the corresponding eigenvectors of the Hamiltonian $\overline{H_0}$ defined in (11), which represents an open N-site chain in the presence of a linear bias of slope $\hbar\phi$. In such a scheme, t plays just the role of an external parameter or an additional coordinate, while the relevant variable defining the dynamical behavior of the Green function is $t - t'$ or, after performing the Fourier transform, the corresponding frequency ω. The integer n in $H_{eff} = H^0_{eff} + H'_{eff}$ runs $-\infty \leq n \leq \infty$.

This redefinition of the problem is equivalent to that introduced by Shirley [24,25] to solve the Schrödinger equation of a time-periodic Hamiltonian by recourse to Floquet theorem. The label n corresponds to the Floquet modes, which appear in the latter theory as a consequence of the periodic nature of the time-dependence of the original Hamiltonian. From the physical point of view we must relate these modes in our problem with the existence of Bloch oscillations. We can borrow the analysis performed in reference [24] and compare the effective Hamiltonian H_{eff} with the Hamiltonian of electrons in interaction with some quantized field. One can distinguish two main differences: (i) The range of n is $0 \leq n \leq \infty$ and (ii) the off diagonal matrix elements $T_{1N} \propto \sqrt{n}$ for the case of a quantized field. Since both differences become small for a large number of quanta, the states $|n\rangle$ can be identified with some quantized field with a large number of quanta carrying each an energy quantum $\hbar\Phi/\Phi_0$. Given this analogy between the Dyson equation at fixed t, and the problem of electrons coupled to some quantized field, we are led to understand the larger conductance in the case of the Kubo geometry as originated by the tunneling of the electrons through the bond $\langle 1, N\rangle$ assisted by the coupling to the quantum modes associated with the Bloch oscillations.

We also analyzed the more general situation indicated in Figure 2, which corresponds to a geometrical arrangement similar to that used to define Kubo conductance, but with a constriction. The difference between the two chemical potentials is $\mu_\beta - \mu_\alpha = \hbar\phi$, which corresponds to the matching condition $\mu^{eff}_\beta - \mu^{eff}_\alpha = \hbar\Phi/\Phi_0$, as explained in Section 2.2. Results are shown in Figure 4 for the cases $T' = T$ (perfect ring) and $T' = 0.1T$ (ring with constriction). These boundary conditions, allow for the flow of current between the ring and the reservoirs, which, for the case of the perfect ring, results in a larger current J along the wire in comparison to the case of Kubo boundary conditions. The fact that J for these boundary conditions is significantly larger than J_L is in agreement with the idea of assisted tunneling as a mechanism to increase the dc-component of the current. Note that a constriction in the system implies a weaker coupling between the electrons and the Floquet quanta which results in a response very close to that obtained for the Landauer geometry.

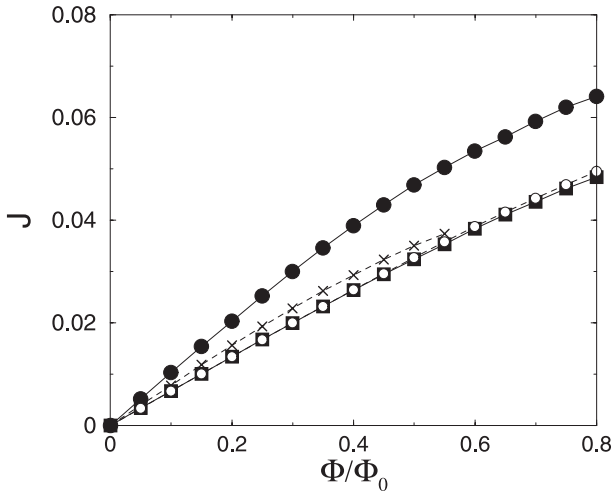

Fig. 4. Currents along the wire for the boundary conditions of Landauer geometry $\mu_\beta - \mu_\alpha = \phi$ for $T' = T$ (filled circles) and $T' = 0.1T$ (filled squares) in a chain with $N = 200$ sites, $\sigma = 0.8T$ and $\mu_\alpha = -T$. J_L and J_K are indicated in open circles and crosses for comparison.

To gain more insight on the role of the Floquet modes let us examine the structure of the transmission functions $T(t, \omega, \Delta)$ and $T_L(\omega, \Delta)$. The behavior of these two functions is strikingly different and is illustrated in Figure 5. The most relevant features to note are: (i) $T_L(\omega, \Delta)$ is always a positive function and exhibits peaks at frequencies corresponding to the energy levels of the uncoupled wire (eigenvalues of $\overline{H_0}$), with a width due to the coupling to the leads. It is quite straightforward to associate this function with the probability for the electrons to be transmitted from one lead to the other when a chemical potential difference eV is established between them. Instead, $T(t, \omega, \Delta)$ can be negative as well as positive, while it exhibits a very complicated structure of peaks. The latter effect is a result of the coupling to the Floquet modes, which originate exchange of spectral weight between different levels of $\overline{H_0}$. For very slow variations of the magnetic flux, the energy quantum $\hbar\Phi/\Phi_0$ is smaller than the typical energy difference between the levels of $\overline{H_0}$ and the structure related to them appears as peaks that are regularly spaced in energy by the amount $\hbar\Phi/\Phi_0$. This is better appreciated in the behavior of the integrated weight

$$I(t, \Delta) = \int_{-\infty}^{+\infty} d\omega T(t, \omega, \Delta), \qquad (25)$$

as shown in the upper panel of Figure 6. In this figure, the integrated weight corresponding to $T_L(\omega, \Delta)$ is also shown for two different values of Φ/Φ_0. In Kubo setup, the

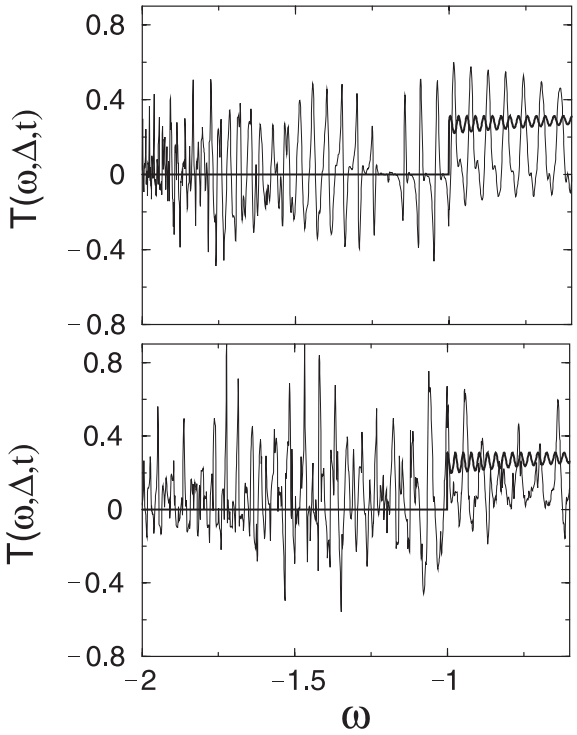

Fig. 5. The transmission function $T(\omega, \Delta, t = 0)$ for a ring of $L = 200$ sites with $\sigma = 0.8T$ and $\mu_\alpha = -T$ The upper (lower) panel corresponds to $\hbar\Phi/\Phi_0 = 0.05T$ ($\hbar\Phi/\Phi_0 = 0.3T$), respectively. The plots in thick lines correspond to the transmission function $T_L(\omega, \Delta)$ for the equivalent parameters.

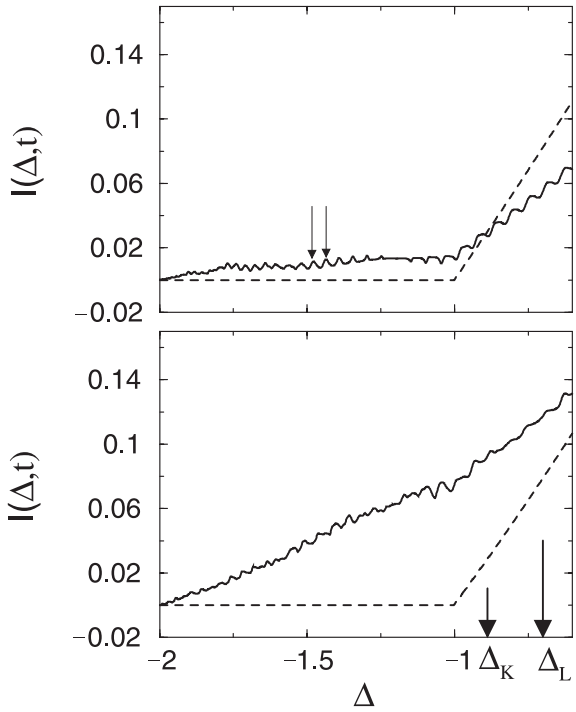

Fig. 6. The integrated weight $I(\Delta, t = 0)$ for the plots of Figure 5. The dashed line corresponds to Landauer geometry. The arrows in the upper panel indicate some of the features regularly spaced in Φ/Φ_0 corresponding to the Floquet modes. The arrows in the lower panel indicate Δ_L (large arrow) and Δ_K (small arrow).

current along the wire is proportional to the time-average of $I(t, \Delta_K)$, with $\Delta_K = \hbar^{-1}eV + \Phi/\Phi_0$, where eV is fixed to obtain a vanishing current along the leads (cf. inset of Fig. 3). In the case of the generalized configuration with constriction, the current along the wire is proportional to the time-average of $I(t, \Delta_L)$, with $\Delta_L = \Phi/\Phi_0$. The current in Landauer setup is proportional to the integral of $T_L(\omega, \Delta_L)$. (ii) The other issue worth to be mentioned is that $T_L(\omega, \Delta)$ is exactly zero for $\omega < \mu_\alpha$. This reflects the fact that in Landauer picture, the only levels of the small system that contribute to the flow of charge are those with energies lying between the two chemical potentials. Instead, $T(t, \omega, \Delta)$ have nonvanishing weight even for $\omega < \mu_\alpha$, and its integration contributes to the finite time-dependent current along the ring, as shown in Figure 6. The time-average of this current has a nonvanishing dc-component. This behavior is due to the fact that in this kind of geometry only one lead (i.e. only one external chemical potential) is enough to generate a finite dc-current along the ring, since the driving force is the induced electric field, while the only role played by the lead is to provide a channel for the dissipation of energy [21].

Increasing (decreasing) the size of the system, it is obtained a similar pattern for the transmission functions with more (less) peaks. The width of the peaks is changed by changing σ, which depends on the strength of the contact and the bandwidth of the leads. The change of these parameters would not modify significantly the basic behavior of $T(t, \omega, \Delta)$. We want to stress that, although the current through the wire is related to the time-average of $I(t, \Delta)$, we have considered a situation with a rather important strength of dissipation σ (note the sizable width of the peaks in Fig. 5). Since dissipation tends to wipe out the time-dependent features of $T(t, \omega, \Delta)$, the data shown in Figures 5 and 6 is representative of the behavior of the time-averaged functions.

We also recall that the calculation of the Kubo current and the current in the more general situation analyzed in Figure 4 when $T' = T$, differ just in the values adopted by Δ (Δ_K and Δ_L, respectively), due to the different boundary conditions chosen in each case. So, the origin of the large magnitude of the current, in comparison to that obtained in Landauer setup is the same in both cases, namely, the peculiar behavior of the transmission function due the coupling between the electronic degrees of freedom and the effective Floquet modes. The situation is, instead, different for the case of the ring with a constriction (also shown in Fig. 4). The behavior of the transmission function and the integrated weight is shown in Figure 7 for $T' = 0.1T$. It can be seen that $T(t, \omega, \Delta)$ is quite close to the transmission function $T_L(\omega, \Delta)$ and that the integrated weight $I(t, \Delta)$ is essentially the same as in the case of Landauer geometry.

To close this section, we analize the behavior of the dissipated power. In reference [16], this quantity has been calculated within first order perturbation theory for the case

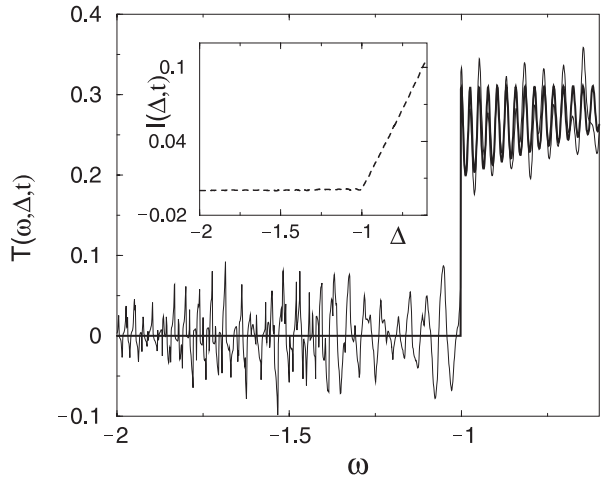

Fig. 7. The transmission function $T(\omega, \Delta, t = 0)$ and the integrated weight $I(\Delta, t = 0)$ (inset) for a ring with a constriction $T' = 0.1T$, $L = 200$ sites, $\sigma = 0.8T$, $\hbar\Phi/\Phi_0 = 0.3T$ and $\mu_\alpha = -T$. The transmission function $T_L(\omega, \Delta)$, corresponding to Landauer setup, is plotted with thick lines in the main panel.

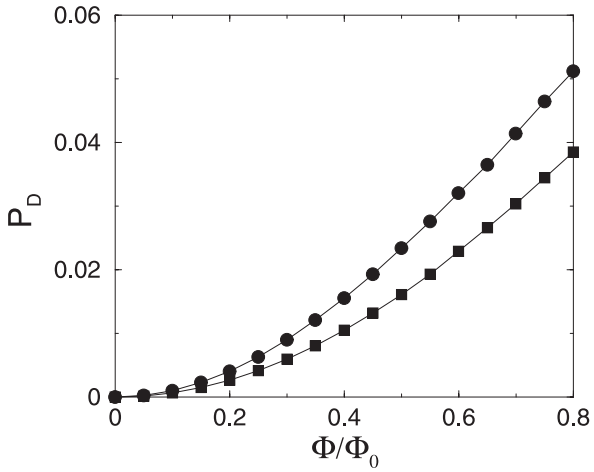

Fig. 8. Dissipated power. The parameters and boundary conditions are the same as in Figure 4.

of a field with an harmonic time-dependence. However, the limit of zero frequency corresponding to the case we study here has not been considered and the explicit functional relation between this quantity and the electric field and induced current has not been analyzed. In Figure 8 we show the dissipated power as a function of Φ/Φ_0 computed from equations (21) and (22). We have verified in all the calculations that $P_D = \sum_l P_D^l$, with $P_D^l = J_{l,l+1}\hbar\phi$. After noting that the electric field is $E = \hbar\phi/a$, we identify the typical form for the dissipated power due to the Joule effect. This provides a nontrivial check of the numerical precision and consistency of our approach.

4 Summary and conclusions

We considered a simple mesoscopic wire of noninteracting electrons and studied its transport properties. We analyzed different geometrical configurations in order to compare the predictions of the two popular Landauer and Kubo definitions for the conductance. Resistive effects were included by coupling the wire to leads in contact with external particle reservoirs. We used a theoretical approach based in Baym-Kadanoff-Keldysh non-equilibrium Green functions. We computed the currents through the different pieces of the circuit and the dissipated power independently. We have verified that the latter is proportional to the dc-component of the current and to the induced electric field, thus obeying the typical law for the Joule effect.

We found that the current through the wire in the Kubo geometry is larger than the Landauer current. We explained this difference as caused by the coupling of the electrons with the effective "quanta" originated by the time-periodic structure of the Hamiltonian in the Kubo case. These effective "quanta" are equivalent to the Floquet modes defined in some theoretical approaches to solve the Shrödinger equation with time-periodic Hamiltonians. In our case, we relate them with the existence of Bloch oscillations. The coupling of the electrons with these modes provide a mechanism for assisted tunneling which results in a larger current in comparison to that obtained with the Landauer setup under the same conditions of applied voltage and dissipation strength. Even sizable, the difference between both currents is not very large. Other ingredients present in more realistic systems, like electron-electron interactions and or electron-phonon interactions, and further dissipative channels, would contribute to break the coherence in the electronic propagation. This would cause an effective weaker coupling between the electrons and the Floquet modes, which would yield to the same response in the two geometries. However, for small and clean wires at low temperatures, within the scale where the electronic coherence is maintained, Bloch oscillations should be observed in the Kubo geometry [21] and the dc-component of the current should differ from that predicted by Landauer formula. Our results are in agreement with those of previous works [18] where Kubo response was defined in a similar experimental condition to that considered in the present work.

There are still some important issues left to the future. One point is a detailed study of the effect of interactions and additional degrees of freedom like phonons. The other fundamental point is related with the energy dissipation: According to our intuition we would expect the wire to heat the environment and to have some high "temperature" and it is interesting to investigate the possibility of defining this concept in some effective way.

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Appendix A: Calculation of the retarded Green functions

We formally separate the problem as indicated in (11), by defining an "unperturbed" part $\overline{H}_0$ that describes an open tight-binding chain plus a "perturbation" $\overline{H}_{1,N}(t)$ corresponding to the time-dependent hopping between the first and the last sites of the chain. Following the procedure of reference [21], it is shown that the final equation for the retarded Green function can be written as

$$\overline{G}^R_{m,n}(t,\omega) = G^0_{m,n}(\omega) - \overline{G}^R_{m,N}\left(t,\omega+\frac{\Phi}{\Phi_0}\right) \times T_{N1}(t)G^0_{1,n}(\omega) - \overline{G}^R_{m,1}\left(t,\omega-\frac{\Phi}{\Phi_0}\right)T_{1N}(t)G^0_{N,n}(\omega), \tag{26}$$

with

$$\begin{aligned}
&\overline{G}^R_{m,1}(t,\omega) + \overline{G}^R_{m,N}\left(t,\omega+\frac{\Phi}{\Phi_0}\right)T_{N1}(t)G^0_{1,1}(\omega) \\
&\quad + \overline{G}^R_{m,1}\left(t,\omega-\frac{\Phi}{\Phi_0}\right)T_{1N}(t)G^0_{N,1}(\omega) = G^0_{m,1}(\omega) \\
&\overline{G}^R_{m,N}(t,\omega) + \overline{G}^R_{m,N}\left(t,\omega+\frac{\Phi}{\Phi_0}\right)T_{N1}(t)G^0_{1,N}(\omega) \\
&\quad + \overline{G}^R_{m,1}\left(t,\omega-\frac{\Phi}{\Phi_0}\right)T_{1N}(t)G^0_{N,N}(\omega) = G^0_{m,N}(\omega).
\end{aligned} \tag{27}$$

For each time t, the solution of the above set of linear equations provides the complete exact solution of the problem. The set (27) involves in principle an infinite number of equations. In the numerical solution, a cutoff for the energy is assumed. Since the spectrum corresponding to $\overline{H}_0$ is bounded, the upper (lower) cuttof is typically assumed to be bigger (smaller) than the highest (lowest) eigenenergy E_ν.

The equilibrium Green function $G^0_{m,n}(\omega)$ corresponds to the problem of an open chain in contact with the reservoirs. It is obtained from the solution of the Dyson equation

$$G^0_{m,n}(\omega) = g^0_{m,n}(\omega) + G^0_{m,1}(\omega)\Sigma_1(\omega)g^0_{1,n}(\omega) + G^0_{m,N}(\omega)\Sigma_N(\omega)g^0_{N,n}(\omega), \tag{28}$$

where

$$g^0_{m,n}(\omega) = \sum_{\nu=1}^{N} A^\nu_m A^\nu_n \frac{1}{\omega - E_\nu + i\eta} \tag{29}$$

with $\eta = 0^+$ is the Green function of the unconnected chain, which can be expressed in terms of the eigenvalues E_ν and eigenvectors $|\nu\rangle = \sum_l A^\nu_l |l\rangle$ of $\overline{H}_0$.

Appendix B: Landauer formula

The geometrical configuration for the evaluation of Landauer conductance corresponds to $T' = 0$. In this case, the current flowing through the system is the same as that flowing through the connecting lead ($J_{1\alpha} = J_{l,l+1}$) while the set of equations for the retarded Green function reduces to $\overline{G}^R_{m,n}(t,\omega) = G^0_{m,n}(\omega)$. From (28) it is easy to prove that

$$\mathrm{Im}\left[G^0_{1,1}(\omega)\right] = \sigma\left(\left|G^0_{1,1}(\omega)\right|^2 + \left|G^0_{1,N}(\omega)\right|^2\right), \tag{30}$$

which when replaced in (12) leads to the Landauer formula (17).

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