Landauer transport as a quasi-steady-state on finite chains under unitary quantum dynamics

J. P. Santos Pires,1,* B. Amorim,2,† and J. M. Viana Parente Lopes1,‡

1Centro de Física das Universidades do Minho e Porto Departamento de Física e Astronomia, Faculdade de Ciências, Universidade do Porto, 4169-007 Porto, Portugal
2Centro de Física das Universidades do Minho e Porto University of Minho, Campus of Guimarães, 4710-057, Braga, Portugal

In this paper, we study the emergence of a Landauer transport regime from the quantum-mechanical dynamics of free electrons in a disordered tight-binding chain, which is coupled to finite leads with open boundaries. Both partitioned and partition-free initial conditions are analyzed and seen to give rise, for large enough leads, to the same spatially uniform quasi-steady-state current, which agrees with the Landauer value. The quasi-steady-state regime is preceded by a transient regime, which last for a time proportional to the length of the disordered sample, and followed by recursions, after a time that is proportional to the lead size. We also observe finite-size current oscillations, superimposed on the quasi-steady-state, whose behavior depends crucially on the conditions initially imposed on the system. Finally, we show how a time-resolved Kubo formula is able to reproduce this Landauer transport regime, as the leads grow bigger.

I. INTRODUCTION

The study of electronic transport is amongst the main goals of condensed matter physics. In the regime of small length scales and low temperatures, the mesoscopic transport regime, quantum coherence effects play a dominant role in the propagation of electron states. In such a case, transport can no longer be seen as a bulk phenomenon, but instead depends on device-specific details such as the geometry of and nature of the electrodes, as well as the specific distribution of disorder in the sample.

A theoretical description of mesoscopic transport was first developed by Landauer and later generalized by Büttiker. In the now called, Landauer-Büttiker formalism, the problem of stationary mesoscopic transport is recast as a scattering problem, where single-electron states incoming from the leads are transmitted across a central device. The current may then be expressed as a sum over the transmission probabilities of the occupied incoming lead states. In parallel to this work, Caroli applied the non-equilibrium Green’s function formalism of Kadanoff-Baym and Keldysh to the calculation of mesoscopic transport. The obtained expression has a structure similar to the Landauer-Büttiker one, but with the transmission coefficient now expressed in terms of Green’s functions of the central device and spectral functions of the leads. While apparently distinct, the two approaches lead to the same result, as implied by the Fisher-Lee relation between transmission coefficients and Green’s functions (for a detailed proof see Ref.9).

Central to both approaches are the assumptions that the leads attached to the central device are semi-infinite and that the occupation of the incoming single-electron states is determined by independent Fermi energies on each lead. Moreover, both methods are only able to describe steady-state transport.

If one is interested in the transient dynamics and how this steady-state is reached, the matter of what the initial condition of the system are, becomes relevant. At the theoretical level, two initial conditions have been historically considered: (i) In the partitioned approach, the leads and the central device are assumed to be initially disconnected, each being in equilibrium with independent Fermi-levels. This Fermi-level imbalance takes into account the applied bias. Then the leads and the device are suddenly brought into contact allowing a charge current to flow. (ii) In the partition-free approach, the leads are assumed to be connected from the beginning, and in global equilibrium with a common Fermi energy. Then a potential bias between the leads is suddenly applied to the connected system. It has been shown that a steady-state transport regime is reached in both approaches and the current coincides in both cases. Crucial to this result is the fact that the leads have a continuum spectrum (as occurs for semi-infinite leads), which leads to a loss of memory about the initial conditions.

In more recent years, a significant effort was devoted to the study of time-dependent transport and transient dynamics in mesoscopic systems attached to infinite leads. In the work of Pal et al., this assumption was relaxed and time-dependent transport through a quantum-dot connected to two systems with a quasi-continuum spectrum (discrete, but dense), which take the role of finite leads, was considered in the partitioned approach. It was found that even in this case, after transients died-out, a steady-state transport regime across the dot emerges. Previously, Di Ventra et al. also explored this possibility and developed a micro-canonical method to deal with quasi-steady-state transport in finite systems. However, many questions remained to be answered about which finite-size effects arise, the dependence of the current’s dynamics on the initial preparation of the system and also the precise conditions in which one expects the emergence of a transport quasi-steady-state.
in the absence of decoherence mechanisms.

The purpose of the present work is to further explore how a steady-state transport regime emerges from quantum time-evolution in systems with finite, but large leads with open boundaries. By combining numerical and analytical work, we study the time-dependent current dynamics in a prototypical one-dimensional non-interacting tight-binding model with disorder, analyzing in detail how the current dynamics depend on the initial conditions (partitioned vs partition-free) and on the size of the finite leads. We employ both a full quantum time-evolution, starting from both initial conditions, and a time-dependent Kubo formula, for the partition-free approach, to study the time-dependent current upon the sudden connection of the appropriate perturbation. The latter allows us to see rigorously how a linear Landauer-Büttiker formula, involving only quantum transmittances, emerges from an unitary time-evolution in the limit of very large leads.

Finally we remark that, besides its theoretical interest, the present paper may also offer predictions for future experiments. It is well established that the use of fermionic ultra-cold atoms trapped in optical lattices allows a very precise tuning of both the interactions and hopping parameters governing the particles’ motion. As discussed by Chien et al., such atomic gases can be prepared in controlled initial states, far away from thermodynamic equilibrium, but their subsequent dynamics must be studied by taking into account the finite number of particles in the gas. Therefore, the finite and closed nature of the leads we are considering, may actually be a relevant feature for the physics of such systems, thus rendering our “finite-size effects” potentially observable.

where the time-evolution of the non-equilibrium current is systematically analyzed as a function of the bias, the size of the finite leads and the central sample’s disorder and size. Finally, in Sec. V, we provide analytical insight into the numerical results of Sec. IV, by developing a time-dependent Kubo formula for the partition-free approach and expressing it in terms of complex reflection and transmission coefficients of the central sample. In Sec. VI, we discuss the obtained results and conclude the paper.

II. MODEL HAMILTONIAN AND INITIAL CONDITIONS

We will study the current dynamics of non-interacting electrons in a finite one-dimensional tight-binding model, with nearest neighbor hoppings. The tight-binding chain is composed by a total of \( L \) sites, with the central \( L_s \) sites, the sample, having an on-site Anderson disorder and being subject to a constant electric field. The sites outside the sample region form the left and right leads (each with \( L_l = (L - L_s)/2 \) sites), are not disordered and hold a constant electrostatic potential. The will refer to the different regions in the chain as Left Lead (LL), Sample (S) and Right Lead (RL). An illustrative scheme of this setup is shown in Fig. 1. For times \( t > 0 \), the dynamics of the system is governed by the time-independent Hamiltonian

\[
\mathcal{H}(t > 0) = \sum_{n=0}^{L-1} \left( \epsilon_n^d - \epsilon_n^e \right) c_n^d c_n^e \nonumber
\]

\[
- w \sum_{n=0}^{L-2} \left( c_{n+1}^d c_n^e + c_n^d c_{n+1}^e \right),
\]

where \( c_n^d (c_n^e) \) are creation (annihilation) operators for an electron at the chain site \( n \), \( w \) is the nearest-neighbor hopping amplitude, \( c > 0 \) is the fundamental charge and \( \epsilon_n^e \) is the electrostatic potential. According to the previous discussion \( \epsilon_n^e \) has the form

\[
v_n^e = \begin{cases} 
\frac{\Delta V}{2}, & n \in 0, \ldots, L_l - 1 \\
\left( \frac{1}{2} - \frac{n-L_l}{L_s+1} \right) \Delta V, & L_l \leq n < L_l + L_s, \\
- \frac{\Delta V}{2}, & n \in L_l + L_s, \ldots, L 
\end{cases},
\]

where \( \Delta V \) is the applied potential bias, and \( \epsilon_n^d \) is the Anderson on-site potential disorder, which is only present in the sample sites, and are taken as random numbers uniformly distributed inside \([ - \frac{W}{2}, \frac{W}{2} ] \).

We will study the current dynamics in this system both in the partitioned and partition-free approaches. In both cases, the dynamics for \( t > 0 \) are governed by the Hamiltonian of Eq. (1), with only the initial state being different.

In the partitioned approach the initial state if formed by occupied states for the partitioned system, with the

![Figure 1. Scheme of the setup used to simulate the time-dependent LB transport using an one-dimensional sample coupled to finite leads. The red dots stand for the places where there is a disordered potential and the blue curve represents the profile of the externally applied potential. The chain has open boundary conditions. (color online)](image-url)
The occupation of the single-electron states is determined by the independent Fermi levels for each region. Hence, we write \( \varepsilon_{R,L} = \varepsilon_{F} + \Delta V/2 \), \( \varepsilon_{S} = \varepsilon_{F} \) and \( \varepsilon_{RL} = \varepsilon_{F} - \Delta V/2 \), as the chemical potential for the left lead, central sample and right lead, respectively. \( \varepsilon_{F} \) is a reference chemical potential. The initial state is thus described by the reduced density matrix

\[
\rho^P(t = 0) = \sum_{r=LL,S,RL} \sum_{\alpha, \bar{\alpha}} f^P_{r,\alpha,\bar{\alpha}} \left| \Psi^P_{r,\alpha} \right\rangle \left\langle \Psi^P_{r,\alpha} \right|, \tag{7}
\]

where \( \left| \Psi^P_{r,\alpha} \right\rangle \) are the independent single-electron eigenstates of the initial partitioned Hamiltonians belonging to region \( r \), \( \mathcal{H}^P_r \), with an energy \( \varepsilon^P_{r,\alpha} \). At any temperature, the initial occupation of the states is given by the factor

\[
f^P_{r,\alpha,\bar{\alpha}} = f(\varepsilon^P_{r,\alpha} - \varepsilon_F),\]

with \( r = LL, S, RL \) and \( f(\varepsilon) = (e^{\beta \varepsilon} + 1)^{-1} \) being the Fermi-Dirac distribution function. Throughout this work, we will restrict ourselves to the \( T = 0 \) case, where \( f(\varepsilon) = \Theta(\varepsilon) \) and \( \Theta(\varepsilon) \) being the usual Heaviside step-function. The hoppings between the leads and the sample are then suddenly switched on and the time-evolution of these states is generated by the Hamiltonian in Eq. (1).

In the partition-free approach, the contact between the sample and the leads is already established in the initial state, but the bias is not yet applied. Therefore, the initial condition is determined by populating the eigenstates of the partition-free Hamiltonian

\[
\mathcal{H}^P(t = 0) = \sum_{n=0}^{L-1} c_n^\dagger c_n - \sum_{n=0}^{L-2} \left( c^\dagger_{n+1} c_n + \text{h.c.} \right), \tag{8}
\]

up to a commonly defined Fermi energy, \( \varepsilon_F \). This initial state is thus described by the reduced density matrix

\[
\rho^PF(t = 0) = \sum_\alpha f^PF_\alpha \left| \Psi^PF_\alpha \right\rangle \left\langle \Psi^PF_\alpha \right|, \tag{9}
\]

with \( \left| \Psi^PF_\alpha \right\rangle \) being eigenstates of Eq. (8) with an eigenenergy \( \varepsilon^PF_\alpha \). The occupation factor of the states is similarly given by \( f^PF_\alpha = f(\varepsilon^PF_\alpha - \varepsilon_F) \). In this case, the sudden perturbation driving the current is the connection of the bias potential, \( e\nu \), at \( t = 0 \), after which the time-evolution is governed by the Hamiltonian of Eq. (1).

We end this section, by noting that the charge current flowing from site \( n \) to site \( n+1 \), for the Hamiltonian of Eq. (1), is given by

\[
I^n = \frac{e}{i\hbar} \left( c^\dagger_{n+1} c_n - c^\dagger_n c_{n+1} \right). \tag{10}
\]

### III. NUMERICAL METHODS FOR CURRENT EVALUATION

#### A. Time-resolved current from quantum evolution of eigenstates

The dynamics of the system, in the partitioned approach after suddenly switching on the lead-sample hoppings, or in the partition-free approach after suddenly switching on the external bias, is governed by the Hamiltonian Eq. (1). Therefore, in both approaches and for \( t > 0 \), the reduced density matrix of the system evolves according to

\[
\frac{d\rho(t)}{dt} = [\mathcal{H}(t > 0), \rho(t)]. \tag{11}
\]

The solution for this equation, with initial condition given by either Eq. (7) or (9), is given by

\[
\rho(t) = \sum_\alpha f_\alpha \left| \Psi_\alpha(t) \right\rangle \left\langle \Psi_\alpha(t) \right|, \tag{12}
\]

with the single-electron states evolving according to Eq. (1): \( \left| \Psi_\alpha(t) \right\rangle = e^{-\frac{i}{\hbar} \mathcal{H}(t > 0) t} \left| \Psi_\alpha \right\rangle \), with \( \left| \Psi_\alpha \right\rangle \) being the single-electron eigenstates of either \( \mathcal{H}^P(t = 0) \) or \( \mathcal{H}^{PF}(t = 0) \) (with occupation \( f_\alpha \)), for the partitioned and partition-free approaches, respectively.

The expected value of the current as a function of time, is given by

\[
I^n(t) = \frac{e}{i\hbar} \sum_{\alpha \in \text{occupied}} \left( \left\langle \Psi_\alpha(t) \right| n + 1 \right) \left\langle n \left| \Psi_\alpha(t) \right\rangle \right. + \left. \left\langle \Psi_\alpha(t) \right| n \right) \left\langle n + 1 \left| \Psi_\alpha(t) \right\rangle \right) , \tag{13}
\]

where \( \left| n \right\rangle \) represents the state localized at site \( n \). We also used the fact that at \( t = 0 \), \( f_\alpha = 1 \) for initially occupied states and \( f_\alpha = 0 \) for empty states. The above expression, allows us to evaluate the current flowing from site \( n \) to site \( n+1 \) provided we know the time-evolution of the initial single-electron states. Although correct, Eq. (13) is not very convenient from a numerical point of view, since for each initially occupied state, we would have to perform one time-evolution. A more convenient expression is obtained by writing

\[
\left\langle \Psi_\alpha(t) \right| n = \langle \Psi_\alpha | e^{\frac{i}{\hbar} \mathcal{H}(t > 0) t} | n \rangle = \langle \Psi_\alpha | n(-t) \rangle ,
\]

such that instead of evolving the initial eigenstate forwards in time,
we evolve the localize states backwards in time\textsuperscript{27} The current can therefore be expressed as

\[
I^n(t) = \frac{2e}{\hbar} \text{Im} \sum_\alpha \langle n(-t) | \Psi_\alpha \rangle \langle \Psi_\alpha | n + 1(-t) \rangle. \tag{14}
\]

Despite being equivalent to Eq. (13), this last expression allows for a great gain in computational efficiency, as the number of required time-evolutions is reduced from $O(L)$ to only two, for each single-time calculation of the current between sites $n$ and $n + 1$.

Numerically, the time-evolution of the localized states $|n\rangle$, for very large chains is computed efficiently using a polynomial Chebyshev expansion\textsuperscript{28,29} of the time-evolution operator $U(t) = e^{-\frac{i}{\hbar} \mathcal{H} t}$ (for details, see Appendix A). Finally, the single-electron eigenstates of the evolution operator of the occupied states, will be compared with the steady-state current, calculated using the quantum evolution operator $\mathcal{H}$. The functions $\rho_{\text{LL/RL}}(\varepsilon)$ are real-space spectral functions of the unattached leads and $G^{RA}(\varepsilon)$ are the real-space retarded/advanced Green’s function of the central sample, in the presence of the leads. For our particular one-dimensional model, the leads’ spectral functions are matrices with the only non-zero elements between boundary sites, i.e. $\Gamma_{\text{LL/RL}}^{L_i} = \Gamma_{\text{LL/RL}}^{L_i-1} \delta_{\varepsilon} + \Gamma_{\text{LL/RL}}^{L_i+1} \delta_{\varepsilon}$, where $\Gamma_{\text{LL/RL}}^{L_i} = w^2 \rho_{\text{LL/RL}}^{L_i}$. The functions $\rho_{\text{LL/RL}}^{L_i}$ are surface density of states of the leads which may be computed analytically yielding:

\[
T(\varepsilon) = \text{Tr} \left[ G^A(\varepsilon) \cdot \Gamma_{\text{RL}}(\varepsilon) \cdot G^R(\varepsilon) \cdot \Gamma_{\text{LL}}(\varepsilon) \right], \tag{16}
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\]

where $\Gamma_{\text{LL/RL}}^{L_i} = \Gamma_{\text{LL/RL}}^{L_i-1} \delta_{\varepsilon} + \Gamma_{\text{LL/RL}}^{L_i+1} \delta_{\varepsilon}$, where $\Gamma_{\text{LL/RL}}^{L_i} = w^2 \rho_{\text{LL/RL}}^{L_i}$. The functions $\rho_{\text{LL/RL}}^{L_i}$ are surface density of states of the leads which may be computed analytically yielding:
\[
\rho_{\text{LL/RL}}(\varepsilon) = \Theta \left( 4w^2 - \left( \varepsilon \mp \frac{e\Delta V}{2} \right)^2 \right) \times \frac{1}{w^2} \sqrt{4w^2 - \left( \varepsilon \mp \frac{e\Delta V}{2} \right)^2}. \quad (17)
\]

Therefore, the final form for the transmission function reads
\[
T(\varepsilon) = w^4 \rho_{\text{LL}}(\varepsilon) \rho_{\text{RL}}(\varepsilon) |G^R_{L_{\text{if}}-1,L_{\text{f}}+L_s}(\varepsilon)|^2. \quad (18)
\]

For each central sample, the retarded Green’s function in Eq. (18) was calculated by using the well-known recursive Green’s function method \cite{9,31,32}, using the surface Green function of the semi-infinite one-dimensional leads as boundary conditions, as detailed in Appendix B.

IV. NUMERICAL RESULTS AND COMPARISON WITH THE LANDAUER FORMULA

We evaluated the time-dependent current in finite open chains, using the method described in Sec. III A, for both clean and disordered samples and considering both the partitioned and partition-free initial conditions. This current was then compared with the Landauer expression for the steady-state current flowing through the same sample attached to infinite leads, as described in Sec. III B.

As we can see in Fig. (2), three regimes are clearly distinguished for large enough leads: (i) initially, we have a transient regime up to a time \( t_{\text{stab}} \), after which (ii) the current eventually approaches an approximately constant quasi-steady-state value, which last up to (iii) a recurrence time, \( t_s \), after which an inversion of the current occurs.

A. Transient Behavior and Stabilization Times

As one could expect, the transient behavior depends on the initial preparation of the system, being different for the partitioned and partition-free approaches, as evident in Fig. 2. On the one hand, after an initial time, during which the current is approximately zero, the transient fluctuations of the current are much more violent in the partitioned case. These fluctuations kick in after a build-up time, \( t_b \), determined by the propagation of a Fermi-level plane-wave from the lead-sample boundaries to the center of the sample, where the current is being probed. The upper panel of Fig. 3, where the current is now probed at a fixed distance \( L_{\text{meas}} \) from the left lead, confirms this interpretation, as \( t_b \approx v_F^{-1} L_{\text{meas}} \).

On the other hand, for the partition-free setup one observes a monotonous build-up of the current from the beginning, which is due to the local dynamics induced inside the central sample, by the sudden connection of the potential ramp. This build-up phase lasts up to a time \( t_b \approx v_F^{-1} L_{\text{meas}} \), at which the effects of the amplitudes initially on the leads start reaching the point of measurement (represented as vertical lines in Fig. 3) At this time, we also observe small inflections in the current, as indicated by the arrows in the bottom panel Fig. 3. After this initial build-up, the current enters a sample-specific damped oscillatory phase which relaxes towards the appropriate Landauer quasi-steady-state.

In both approaches, after a time which grows with the central sample size, \( t_{\text{stab}} \approx 2v_F^{-1} L_s \), the value of the current stabilizes to an approximately constant value, as shown by the collapse of the curves in Fig. 3, where the time axis is shown in units of \( t_{\text{stab}} \). Physically, this time can be interpreted as the one needed for the quantum single-particle states near \( \varepsilon_F \) to travel back and forth inside the central sample and thus probing the existing disorder landscape. Curiously, this time-scale is roughly independent of the particular disorder configuration in question.

B. Landauer Quasi-Steady-State Transport, Finite-Size Effects and Recurrence Times

In both approaches, if the leads are large enough, the initial build-up and stabilization of the current is fol-
lowed, for \( t > t_{\text{stab}} \), by an intermediate time period where the current through the sample stabilizes. As the size of the leads increases, the value of this quasi-steady-state current tends to the sample-specific Landauer value, independently of the initial preparation of the system (partitioned or partition-free). Hence, the present result are numerical checks of the memory-loss theorem of Stefanucci et al.\(^{13}\). This theorem states that, provided the leads have a continuum spectrum, a steady-state value of the current is achieved for long times and that this value is independent of the initial state of the system.

The bias used was \( \Delta V \) obtained from the Landauer formula with semi-infinite leads. The Fermi energy. The dashed magenta lines correspond, once again, to the respective steady-state current obtained from the Landauer formula with semi-infinite leads. The bias used was \( \Delta V = 0.1w \). (color online)

In our case, a quasi-steady-state only occurs for intermediate times, due to the finite nature of the leads, which makes their spectrum discrete. One expects that for sufficiently large leads, the value of the current in the quasi-steady-state approaches the Landauer value. However, the way in which this occurs depends crucially on the initial condition of the system. In the partition-free approach, we observe that the current in the quasi-steady-state regime does not approach the Landauer value monotonically in time. Instead, there is a small oscillatory component, with approximately constant amplitude in time, superposed on its steady-state value, which persists up to the first recursion time. The amplitude of these oscillations is seen to decrease as \( L_l \to \infty \), which identifies them with a finite-size effect that disappears in the limit of semi-infinite leads. We also observed, that the period of this oscillations is roughly inversely proportional to the applied bias. For the partitioned approach, a rather different behavior is observed. In this setup, the amplitude of the oscillations does not decay as \( L_l \) is increased, being roughly independent of the size of the leads for a fixed observation time. Instead, it is the amplitude of the oscillations that decays over time. As the size of the leads is increased, the quasi-steady-state can be observed for longer times, for which the amplitude of the oscillations is smaller. Despite being roughly independent of \( L_l \) for a fixed observation time, these are also finite-size effects since they only disappear as \( t \to \infty \), hence being limited by the recursion time \( t_r \). All the previous effects are depicted in the four insets of Fig. 2.

Pal et al.\(^{21}\) pointed out that the recurrence time is inversely proportional to the level spacing of the leads’ spectra, which measures how close the finite leads are to a true continuous spectrum. Our present results allow for an alternative interpretation. As demonstrated in Figs. 2 — where we show the current for fixed Fermi energy and different sizes of the leads — and in Fig. 4 — where we show the current for fixed \( L_l \) but different Fermi energies — the recurrence time is roughly given by \( t_r \sim 2v_F^{-1}L_l \), where \( v_F \) is the Fermi velocity. Notice that \( 2v_F^{-1}L_l \) is just the time a Fermi-level electron takes in a round trip inside of a lead, in agreement with what was previously reported in Ref. Bushong et al.\(^{23}\). Furthermore, one also sees that the recursion time is roughly independent of the disorder on the sample, which is consistent with its previous physical interpretation.

Figure 4. Plots of the time-dependent current from the unitary quantum dynamics in the partition-free approach and for a single disordered central sample at different values of the common Fermi energy. The dashed magenta lines correspond, once again, to the respective steady-state current obtained from the Landauer formula with semi-infinite leads. The bias used was \( \Delta V = 0.1w \). (color online)

Figure 5. Plots of the electric current traversing the central bond (blue curves) and the boundaries (red and green curves) of a disordered sample of length \( L_s = 256 \) and disorder strength of \( W = 0.3w \). The leads had a length of \( L_l = 2^{13} \) and a potential difference of \( \Delta V = 0.01w \). The top panel depicts the calculation done with the partitioned setup, while in the bottom panel the partition-free configuration was used. The dashed magenta lines stand for the value of the steady-state current obtained using the Landauer formula for this sample. (color online)

In a true steady-state, the value of the current is not only time-independent but must also position-independent, as no charge accumulation can occur. Hence, we also investigated whether or not this emergent quasi-steady-state current in finite chains is homogeneous over the sample. Indeed, we found out that in
the quasi-steady-state the current is approximately homogeneous in space, independently of the initial preparation of the system, for large enough leads and provided we are far away from the chain’s open extremities. This observation is exemplified in Fig. 5, where we show the time-dependent current for a disordered central sample, measured at three different bonds: center, left and right boundaries of a randomly picked disordered sample. As can be seen, after the disappearance of the initial transients, the same quasi-steady-state current is reached at the three positions, apart from the finite-size oscillations which are different.

![Figure 6. Plots of the time-dependent current across a disordered sample coupled to finite leads with $L_i = 16384$ sites and for different values of $\Delta V \ll w$. The full lines stand for the results of a fully non-linear calculation using the quantum dynamics method of last section in the partitioned (upper panel) and partition-free approach (lower panel), while the points stand for the raw evaluation of the linear response Eq. (28). The last are only present in the partition-free case, where the time-dependent Kubo formula is valid. The value of the current is normalized to the corresponding Landauer steady-state value. (color online)](image)

Interestingly, the establishment of a well defined quasi-steady-state might not occur for very small biases, where we would expect linear response theory to hold, depending on the initial conditions. This is illustrated in Fig. 6. There, we can see that for the partition-free setup, no clear quasi-steady-state is observed for very small biases. This occurs because, for fixed leads size, the period and amplitudes (relative to the infinite leads’ Landauer value) of the finite-size oscillations increases with the applied bias. Therefore, for small enough bias, the period of the oscillations might become larger than the recursion time, and no quasi-steady-state is observed. In the partitioned setup, the situation is a bit different and for large times: the current always tends to the Landauer value with the amplitude of the finite-size oscillations decreasing over time. These observations seem to be in agreement with the interpretation of Ref. Bushong et al.\textsuperscript{23}, where it is put forward that the observation of a quasi-steady-state requires the change in the initial spread of the electrons’ momenta. In Ref. Bushong et al.\textsuperscript{23}, this occurs either due to a geometrical constriction at the lead-sample contact, or due to an initial applied energy barrier. In our case, it seems that the applied bias is the mechanism by which electrons change their initial momenta. As a general “rule-of-thumb”, we can tell that, in order to observe a quasi-steady-state current regime with minor finite-size effects, one must always consider biases that are much larger than the level spacing of the whole system’s spectrum.

C. Sample-Specific $I - V$ curves at large biases

![Figure 7. Plots of the $I (\Delta V)$ curves of two independent disordered samples. The black curves in the main plots were obtained using the Landauer formula of Eq. (18). The red dots were obtained from the quasi-steady-state current of a quantum dynamics calculation, using the partition-free approach with $L_i = 2^{14}$ sites. The use of a partitioned approach could also be done, but would be redundant given that we proved the numerical equivalence of both approaches in the previous discussion. In the insets, we highlight with a red arrow the time of measurement in a plot of $I(t)$. (color online)](image)

This is illustrated in Fig. 7, where we show values for the time-dependent current in the quasi-steady-state...
regime as a function of the applied bias, for two random disordered samples, and compare the results with the value of the Landauer current. The results clearly confirm that the quasi-steady-state current seen in the quantum dynamics calculations with finite leads indeed corresponds to the Landauer transport predicted for samples coupled to semi-infinite leads. The agreement between the two approaches was seen to be perfect for all the range of bias tested and well beyond linear response.

V. EMERGENCE OF LANDAUER TRANSPORT WITHIN LINEAR RESPONSE IN THE PARTITION-FREE APPROACH

The numerical studies of the previous section show that a quasi-steady-state transport regime, with an approximately uniform and time-independent current, emerges across finite systems subjected to a potential bias and coupled to finite but large leads. Moreover, the results also show that for large enough leads, the value of this quasi-steady-state current coincides with the Landauer result for the transport’s steady-state with semi-infinite leads. In this section, we will try to shed further light on these numerical results using a semi-analytical procedure. In order to make as much analytical progress as possible, we shall restrict ourselves to the partition-free case and small biases, such that we can study the current using Kubo linear response theory in the applied bias, $\Delta V$.

A. Time-dependent Kubo formula for a sudden connection

We will always consider the partition-free Hamiltonian at $t = 0$ as the unperturbed Hamiltonian for this case, i.e.

$$\mathcal{H}_0 = \mathcal{H}_0^{PF}(t = 0) = -\sum_{n=0}^{L-1} c_n^{\dagger} c_n - w \sum_{n=0}^{L-2} (c_{n+1}^{\dagger} c_n + c_n^{\dagger} c_{n+1})$$

(19)

and treat the applied potential bias as the current-driving perturbation,

$$\mathcal{V}(t) = -e\Theta(t) \sum_{n=0}^{L-1} v_n^{c}\delta c_n^{\dagger} c_n.$$  

(20)

with the electrostatic potential profile, $v_n^{c}$, given by Eq. (2).

In order to derive a time-dependent Kubo formula for the current, we will start by writing the equation of motion for the reduced density matrix, Eq. (11), in the eigenbasis of the unperturbed Hamiltonian. Thus, we obtain

$$\frac{d}{dt} \rho_{\alpha\beta}(t) = -i \frac{\varepsilon}{\hbar} (\varepsilon_\alpha - \varepsilon_\beta) \rho_{\alpha\beta}(t) - \frac{i e}{\hbar} [\mathcal{V}(t), \rho(t)]_{\alpha\beta}$$

(21)

where $O_{\alpha\beta}(t) = \langle \Psi_\alpha | \mathcal{O} | \Psi_\beta \rangle$ and $| \Psi_\alpha \rangle$ is an eigenstate of $\mathcal{H}_0$ with energy $\varepsilon_\alpha$. Within linear response theory, we write the reduced density matrix as

$$\rho_{\alpha\beta}(t) = \delta_{\alpha\beta} f(\varepsilon_\alpha) + \delta \rho_{\alpha\beta}(t),$$

(22)

where $\rho_{\alpha\beta}(0) = \delta_{\alpha\beta} f(\varepsilon_\alpha)$ is the initial equilibrium reduced density matrix and $\delta \rho_{\alpha\beta}(t)$ is a small correction, which in linear response is assumed to be $\propto \mathcal{V}(t)$. Disregarding any contributions of $\mathcal{O}(\mathcal{V}^2)$ in the equation of motion, we obtain

$$\frac{d}{dt} \delta \rho_{\alpha\beta}(t) = -i \frac{\varepsilon}{\hbar} (\varepsilon_\alpha - \varepsilon_\beta) \delta \rho_{\alpha\beta}(t) - \frac{i e}{\hbar} \Theta(t) \Gamma_{\alpha\beta} (f(\varepsilon_\alpha) - f(\varepsilon_\beta)).$$

(23)

where $\Gamma_{\alpha\beta}$ are the matrix elements of the applied potential bias,

$$\Gamma_{\alpha\beta} = \sum_n \psi_\alpha^*(n) \psi_\beta(n) v_n^{c},$$

(24)

and $\psi_\alpha(n)$ is the amplitude of the eigenstate $| \Psi_\alpha \rangle$ on site $n$, i.e. $\psi_\alpha(n) = \langle n | \Psi_\alpha \rangle$. Now, using the fact that $\delta \rho_{\alpha\beta}(t < 0) = 0$, it is possible to integrate Eq. (23), obtaining

$$\delta \rho_{\alpha\beta}(t) = -e \Gamma_{\alpha\beta} \frac{\Delta f_{\alpha\beta}}{\Delta \varepsilon_{\alpha\beta}} (1 - e^{-\frac{i}{\hbar} \Delta \varepsilon_{\alpha\beta} t}),$$

(25)

where $\Delta f_{\alpha\beta} = f(\varepsilon_\alpha) - f(\varepsilon_\beta)$ and $\Delta \varepsilon_{\alpha\beta} = \varepsilon_\alpha - \varepsilon_\beta$. The expected value of the current that flows from site $n$ to $n + 1$, is thus given by

$$I_n(t) = \frac{i e^2 w}{\hbar} \sum_{\alpha\beta} \Pi_{\alpha\beta} n^\alpha \Gamma_{\beta\alpha} \frac{\Delta f_{\alpha\beta}}{\Delta \varepsilon_{\alpha\beta}} (1 - e^{-\frac{i}{\hbar} \Delta \varepsilon_{\alpha\beta} t}),$$

(26)

where we introduced

$$\Pi_{\alpha\beta} = \psi_\alpha^*(n + 1) \psi_\beta(n) - \psi_\alpha^*(n) \psi_\beta(n + 1),$$

(27)

which are the matrix elements of the local current operator between sites $n$ and $n + 1$, up to a dimension-full multiplicative factor.

By further noticing that the amplitudes $\psi_\alpha(n)$ may be chosen as all real and $\Pi^\alpha$ is an anti-symmetric matrix, one can rewrite Eq. (26) in the following way:

$$I_n(t) = \frac{2 e^2 w}{\hbar} \sum_{\alpha\beta} \sum_{\varepsilon_\alpha \leq \varepsilon_\beta} \Pi_{\alpha\beta} n^\alpha \frac{\sin \left( \frac{\Delta \varepsilon_{\alpha\beta} t}{\hbar} \right)}{\Delta \varepsilon_{\alpha\beta}},$$

(28)

which is our final time-dependent Kubo formula for the current.

Obviously, one cannot give a general rule for establishing the validity regime of Eq. (28), since that will depend crucially on the properties of the central disordered sample. However, for each sample, there is always a value of $\Delta V$ sufficiently small, such that a linear response theory for the current is valid. We depict such an example in the upper panel of Fig. 6, where the current traversing the central bond of a disordered sample, as obtained from Eq. (28), is compared with the one obtained from the fully
nonlinear quantum dynamics of sec. III in the partition-free approach. As a further short comment on the plots of Fig. 6, it is interesting to note that, for the parameters used, it seems that no quasi-steady-state plateau emerges from the quantum dynamics close to the linear response regime. As referred before, this is simply a consequence of a greater relevance of the finite-size oscillations which, now, have a period larger than the recurrence time and a much larger relative amplitude.

B. Representation of the eigenstates in terms of the sample’s quantum reflection/transmission coefficients

In order to make an effective use of Eq. (28) and make analytic progress we must be able to find a semi-analytical expression for the matrix elements $\Pi_{\alpha \beta}$ and $\Gamma_{\alpha \beta}$, which, in principle, requires the knowledge of the eigenfunctions in the whole chain. These wavefunctions usually present a very complicated structure inside the disordered central sample, but for large enough leads, we actually only need to know their form in the leads. On the one hand, the $\Pi_{\alpha \beta}$ matrix elements only require the knowledge of local amplitudes in the two adjacent sites across which the current is being measured. Hence, we can simply choose to measure it outside the sample. On the other hand, we expect the current to be dominated by states that are not localized in the disordered sample, but instead are delocalized in the leads. Hence, we only need to calculate the $\Gamma_{\alpha \beta}$ matrix elements between delocalized states. For such states, and provided the leads are much larger than the disordered sample region, we can approximate

$$\Gamma_{\alpha \beta} = \sum_n \psi_\alpha^*(n)\psi_\beta(n)\phi_n \simeq \sum_{n \in \text{Leads}} \psi_\alpha^*(n)\psi_\beta(n)\phi_n. \quad (29)$$

This approximation, allows us to evaluate the current $I^\alpha(t)$ in the leads, without knowing the shape of the eigenfunctions inside the central sample.

Next, we notice that the form of the scattering eigenstates in the leads can be expressed in terms of the complex reflection and transmission coefficients of the central sample. For perfect leads, the wavefunctions of the eigenstates will have the form of a coherent superposition of left and right propagating plane-waves. With a change of notation from the previous section, we will relabel sites of the left lead with indices $n = -L_1, ..., -1$ and the ones of the right lead with $n = 1, ..., L_1$. Using this notation, the form of the eigenstate wavefunction $|\Psi_k\rangle$ in the leads have the form

$$\psi_k(n) = \langle n | \Psi_k \rangle = \begin{cases} \Psi_L e^{ik(n-1)} + \Psi_R e^{-ik(n-1)}, & -L_1 \leq n \leq -1 \\ \Psi_L e^{ik(n-L_1)} + \Psi_R e^{-ik(n-L_1)}, & 1 \leq n \leq L_1 \end{cases}, \quad (30)$$

being labeled by a crystal momentum $k$, and with $\Psi_{L/R}^\pm(n)$ being the amplitude of a right/left propagating state in the left (right) lead. Notice that the time-independent Schrödinger equation inside the leads, still allows us to relate the crystal momentum $k$ to the energy of the state as $E = -2t \cos(k)$, i.e. the same as for an infinite periodic chain. As usual in one-dimensional scattering problems, the amplitudes of propagating states on the left and right leads can be related by a transfer matrix, $\mathcal{M}(k)$:

$$\begin{pmatrix} \Psi_R^k \\ \Psi_L^k \end{pmatrix} = \mathcal{M}(k) \cdot \begin{pmatrix} \Psi_L^- \\ \Psi_R^- \end{pmatrix}, \quad (31)$$

In the presence of time-reversal symmetry, the transfer matrix has the general form

$$\mathcal{M}(k) = \begin{pmatrix} \frac{1}{|t(k)|} e^{i\theta(k)} & \frac{|t(k)|}{|\Gamma(k)|} e^{-i\phi(k)} \\ \frac{|r(k)|}{|\Gamma(k)|} e^{i\phi(k)} & \frac{1}{|r(k)|} e^{-i\theta(k)} \end{pmatrix}, \quad (32)$$

where $|t(k)|/|r(k)|$ and $\phi(k)/\theta(k)$ are the moduli and phases of the transmission/reflection coefficients, respectively. Moreover, for any sample one has det $\mathcal{M} = 1$, which implies the conservation of current, i.e. $|t|^2 + |r|^2 = 1$. These coefficients are physical characteristics of the central sample only and, thus, may be rightfully calculated by assuming the leads as semi-infinite. The determination of the reflection and transmission coefficients of a specific sample, in general, can only be done numerically, using the method detailed in Appendix B. The great advantage of this method is that, once this calculation is done, the wavefunctions in the leads can be expressed in terms of only a few parameters. Additionally, to obtain the eigenstates, we must further impose open boundary conditions at the ends of the leads, i.e.

$$\psi_k(-L_1 - 1) = \psi_k(L_1 + 1) = 0. \quad (33)$$

Combining Eqs. (30)-(33) one arrives at the following general expression for the wavefunctions:

$$\psi_k(n) = \frac{1}{\sqrt{N_k}} \begin{cases} |t(k)| \sin \left( n \left( k + L_1 + 1 \right) \right) & n < 0 \\ f_2(k) \sin \left( n \left( k - L_1 - 1 \right) \right) & n > 0 \end{cases}, \quad (34)$$

where $N_k$ is a normalization factor, which can be determined in the limit of large leads by approximating, in the same spirit of Eq. (29),

$$\sum_n |\psi_k(n)|^2 \simeq \sum_{n \in \text{Leads}} |\psi_k(n)|^2. \quad (35)$$

This finally leads to

$$N_k \simeq L_1 f_1(k). \quad (36)$$

The functions $f_1(k)$ and $f_2(k)$ are defined as

$$f_1(k) = 1 + |r(k)| \cos \left( 2k(L_1 + 1) + \theta(k) \right) \quad (37a)$$

$$f_2(k) = \cos \left( 2k(L_1 + 1) + \phi(k) \right) + |r(k)| \cos \left( \theta(k) - \phi(k) \right), \quad (37b)$$

and where $k$ is constrained to verify the following quantization condition:
\[
\sin \left[ 2k (L_l + 1) + \phi (k) \right] = |r (k)| \sin \left[ \theta (k) - \phi (k) \right].
\]  

Notice that the solution of this last condition, together with the relation \( k = \arccos (-E / 2w) \), allows us to determine the eigenenergies corresponding to delocalized states. In the lower panels of Fig. 8 (b), we exemplify the validity of this statement by comparing the wavefunctions obtained from the numerical diagonalization of \( H_0 \), with \( L_l = 8192 \) sites, to the semi-analytical expressions of Eq. (34). The wavenumbers obtained from the numerical diagonalization, i.e. \( k = \arccos (-E/2) \), are also seen to coincide perfectly with the roots of Eq. (38) (see the upper panels of Fig. 8 (b)).

Note also that Eqs. (34) and (38) reduce to the usual result for the eigenstates of a finite open chain, when \( |r (k)| = 0 \) and \( \phi (k) = k (L_l - 1) \) is the phase accumulated by a plane-wave crossing the internal bonds of an ordered sample, i.e.

\[
\psi_k (n) = \frac{1}{\sqrt{L_l}} \begin{cases} 
\sin \left[ k (n + L_l + 1) \right], & n < 0 \\
(-1)^p \sin \left[ k (n - L_l - 1) \right], & n > 0
\end{cases}
\]  

(39)

with \( k = \pi p / (L + 1) \) and \( p = 1, ..., L \). Moreover, these states are non-degenerate and also alternately symmetrical and antisymmetrical under parity \( (n \rightarrow -n) \), which just reflects that same symmetry of the clean Hamiltonian.

With the knowledge of the eigenstates wavefunctions of the leads, Eq. (34), we can write the matrix elements \( \Gamma_{k,q} \) and \( \Pi^n_{k,q} \). With the approximation of Eq. (29), we can evaluate \( \Gamma_{k,q} \) analytically, obtaining

\[
\Gamma_{k,q} \simeq \Delta V \left| \frac{|t (k)||t (q)| - f_2 (k) f_2 (q)}{8L_l \sqrt{f_1 (k) f_1 (q)}} \right| \times \\
\times \left\{ \sin \left[ \frac{(q-k)(L_l+1)}{2} \right] - \sin \left[ \frac{(q+k)(L_l+1)}{2} \right] \right\}.
\]  

(40)

As for the matrix elements \( \Pi^n_{k,q} \), from the definition Eq. (27), for bonds in the left lead \( n < -1 \), and after some simple manipulations, we obtain

\[
\Pi^n_{k,q} \simeq 1 = \frac{|t (k)||t (q)|}{L_l \sqrt{f_1 (k) f_1 (q)}} \times \\
\times \left\{ \sin \left( \frac{k-q}{2} \right) \sin \left[ (k+q) \left( n + L_l + \frac{3}{2} \right) \right] - \sin \left( \frac{k+q}{2} \right) \sin \left[ (k-q) \left( n + L_l + \frac{3}{2} \right) \right] \right\}.
\]  

(41)

while for the current in bonds of the right lead \( n > 1 \), we obtain a similar result after replacing \( |t (k)||t (q)| \rightarrow f_2 (k) f_2 (q) \) and \( L_l \rightarrow -L_l - 2 \) in Eq. (41).

C. The continuum regime of the Kubo formula

When analyzing the time-dependent Kubo formula of Eq. (28), we must take into account that there are actually two distinct time scales: 1) the observation time, \( t \), and 2) the scale associated with the spacing between the discrete energy levels of the finite chain. The latter is proportional to the length of the leads and, as discussed in the Sec. IV, is associated to the recurrence time \( t_r \sim 2L_l/vF \).

As expected and confirmed in Sec. IV, the quasi-steady-state regime which approximates the Landauer
transport regime of semi-infinite leads, emerges when we take \( T, L_1 \to \infty \) (with \( T = t \omega / \hbar \) being the time in dimensionless units), but while keeping \( T \ll L_1 \). In such case, all the transients have died out, but the system is still far away from getting into the regime where current inversions occur. Furthermore, Eq. (28) includes a factor of \( \sin (\Delta \varepsilon_{\alpha \beta} t / \hbar) / \Delta \varepsilon_{\alpha \beta} \), which is an emergent \( \delta \)-function in the limit \( t \to +\infty \), with a broadening of \( \hbar t^{-1} \) in energy. This factor actually acts as a spectral filter which kills-off the contributions coming from pairs of eigenstates having an energy separation larger than \( \hbar t^{-1} \). Hence, we will show in this section how the approximately time-independent quasi-steady-state current emerges, when we are in the limit \( T, L_1 \to \infty \), with \( T \ll L_1 \), such that there are many eigenvalues inside the interval \([\varepsilon_F - \hbar t^{-1}, \varepsilon_F + \hbar t^{-1}]\). We will refer to this limit as the \textit{continuum regime}.

1. \textit{Approximate form of \( \Gamma_{k,q} \) and \( \Pi^\sigma_{k,q} \) matrices in the \textit{continuum regime}}

We start by noting that, in the continuum limit, since only states close to the Fermi energy contribute, it sufficient to obtain the matrix elements \( \Gamma_{k,q} \) and \( \Pi^\sigma_{k,q} \) between states where \( k - q \) is small and \( k, q \simeq k_F \). In the limit of \( k - q \to 0 \), the first term of Eq. (40) dominates over the second. Therefore, we can approximate it as

\[
\Gamma_{k,q} \simeq \Delta V \frac{|t(k)| |t(q)| - f_2(k) f_2(q) \sin (k - q) L_1}{8 L_1 f_1(k) f_1(q) \sin \left( \frac{k-q}{2} \right)},
\]

where, in the of limit \( L_1 \to \infty \), we approximated \( [(q-k)(L_1 + \frac{1}{2})] \simeq \sin [(q-k) L_1] \). Doing the same for \( \Pi^\sigma_{k,q} \), we obtain

\[
\Pi^\sigma_{k,q} \simeq -\frac{|t(k)| |t(q)|}{L_1 f_1(k) f_1(q)} \sin (k_F) \sin [(k-q) L_1],
\]

where we assumed that \(|n| \ll L_1 \), when approximating \( [(k-q)(n+L_1+\frac{1}{2})] \simeq \sin [(k-q) L_1] \). This justifies why in the quasi-steady-state regime, the current is approximately uniform, if we are away from the chain’s extremities. For the current on the right lead, we obtain a similar result, namely,

\[
\Pi^\sigma_{k,q} \simeq \frac{f_2(k) f_2(q)}{L_1 f_1(k) f_1(q)} \sin (k_F) \sin [(k-q) L_1].
\]

Now, we note that for a chain without any disorder, the matrix elements of \( \Gamma_{k,q} \) will only be non-zero if the states labeled to \( k \) and \( q \) have opposite parities. This selection rule stems from the fact that the fully ordered chain is symmetric under inversion and therefore its eigenstates will have a well-defined parity. Since the applied potential \( \nu_n \) is an odd perturbation, it only couples states of opposite parities. In the presence of a general disorder in the central sample, we no longer have inversion symmetry. Nevertheless, one may still expect that in the limit \( L_1 \gg L_s \), the breaking of the symmetry is small and an approximate selection rule should emerge. Indeed, this is the case. In order to obtain this approximate selection rule for a sample with disorder, we notice that although we can no longer classify the states as even and odd, given the quantization condition Eq. (38), which involves \( \sin [2k(L_1+1) + \phi(k)] \), we can classify the states as + and - according to the sign of \( \cos [2k \tilde{L}_1 + \phi(k)] \):

\[
\cos [2k \tilde{L}_1 + \phi(k)] = \pm \sqrt{1 - |r(k_F)|^2 \sin^2 (\theta(k_F) - \phi(k_F))}. \text{ (45)}
\]

For an ordered or symmetrically disordered sample, this reduces to a labelling of eigenstates as even or odd, respectively, under a parity transformation, \( n \to -n \). With such a classification, it can be shown (see Appendix C) that in the limits of \( k-q \to 0 \) and \( L_1 \to \infty \), one obtains the following effective selection rule:

\[
\lim_{L_1 \to \infty} \left| \sin \left( \left( k^\sigma - q^{\sigma'} \right) \tilde{L}_1 \right) \right| = (1 - \delta_{\sigma,\sigma'}) \times \\
\frac{\sqrt{1 - |r(k_F)|^2 \sin^2 (\theta(k_F) - \phi(k_F))}}{1 \pm \sqrt{1 - |r(k_F)|^2 \sin^2 (\theta(k_F) - \phi(k_F))}}. \text{ (46)}
\]

We point out that in the case of symmetric disorder profile, one can derive from the properties of the transfer matrix that \( \phi(k)-\theta(k) = \pm \pi/2 \). In this case, one immediately sees that the scattering wavefunctions of Eq. (34) reduce to the same form as in Eq. (39), with the parity determined by the class to which it belongs. In such a case, the \( |t(k)| \) factor of the \( \Gamma \) and \( \Pi^\sigma \) matrices comes only from this effect, since the functions \( f_1(k) \) and \( f_2(k) \) are exactly the same as in the non-disordered case. Just the allowed \( k \)'s are different.

Having established this effective selection rule, we can expand the prefactors of Eqs. (42)-(44) around \( k_F \). Taking into account that the only significant contributions come from pairs of states belonging to different classes, we may use Eqs. (38) and (45) to write, for \( k, q \simeq k_F \),

\[
f_1(k) f_1(q) \simeq \left( 1 - |r(k_F)|^2 \sin^2 (\theta(k_F) - \phi(k_F)) \right) |t(k_F)|^2, \text{ (47a)}
\]

\[
f_2(k) f_2(q) \simeq -|t(k_F)|^2. \text{ (47b)}
\]
Using these approximations in Eq. (42), we obtain
\[ \Gamma_{k,q} \simeq \Delta V \frac{|t(k_F)|}{4L_f} \frac{1}{\sin \left( \frac{k-q}{2} \right)} \]
\[ \simeq \Delta V \frac{|t(k_F)|}{2L_f} \frac{1}{k-q}, \] (48)
and from Eqs. (43)-(44) we obtain
\[ \Pi_{k,q}^\downarrow \simeq \Pi_{k,q}^\uparrow \sim -\frac{|t(k_F)|}{L_f} \sin (k_F). \] (49)
In the following, we will use Eqs. (48)-(49) to obtain the Landauer current from the Kubo formula of Eq. (28)

\[ I^n(t) = \frac{e^2}{\hbar} |t(k_F)|^2 (v_F h)^2 \Delta V \]
\[ \times \int_{-\infty}^{+\infty} d(\Delta \varepsilon) \sin \left( \frac{\Delta \varepsilon t}{\hbar} \right) \frac{\sin (\Delta \varepsilon \varepsilon_t/\hbar)}{\Delta \varepsilon} g(\Delta \varepsilon), \] (52)
where we introduced the joint density of contributing states (JDoCS), \( g \), as
\[ g(\varepsilon_F, \Delta \varepsilon) = \frac{1}{4L_f^2} \sum_{k,q} \delta(\Delta \varepsilon - \varepsilon_{k,q}). \] (53)

The restricted summation in Eq. (53) already takes into account the emergent selection rule of Eq. (46). In Appendix D, we show that this quantity, in the limit \( L_i \to \infty \), can be written in terms of the density of states of each class in a fully clean system and its expression for small enough \( |\Delta \varepsilon| \) is simply
\[ \lim_{L_i \to \infty} [g(\varepsilon_F, \Delta \varepsilon)] = \frac{|\Delta \varepsilon|}{2\pi^2 (4w^2 - \varepsilon_F^2)} + O[\Delta \varepsilon^2]. \] (54)
Hence, when Eq. (54) is plugged into Eq. (52), we get
\[ I^n(t) = \frac{e^2}{2\pi^2 \hbar} |t(k_F)|^2 (v_F h)^2 \Delta V \]
\[ \times \int_{-\infty}^{+\infty} d(\Delta \varepsilon) \frac{\sin (\Delta \varepsilon \varepsilon_t/\hbar)}{\Delta \varepsilon}. \] (55)
Finally, Eq. (55) together with the facts that
\[ \lim_{T \to \infty} \left[ \sin \left( \frac{\pi x T}{x} \right) \right] = \pi \delta(x), \] (56)
and \( v_F \hbar = \sqrt{4w^2 - \varepsilon_F^2} \), yields a steady-state current
\[ I^n(t) = \frac{e^2}{\hbar} |t(k_F)|^2 \Delta V, \] (57)
which is precisely the linear Landauer steady-state current for a two-terminal one-dimensional device.

Notice, that in the derivation of this result from the time-dependent Kubo formula, it is essential that \( t, L_i \to \infty \) with \( wt/\hbar \ll L_i \), such that the \( g(\Delta \varepsilon) \) can be evaluated in the limit of \( L_i \to \infty \), while the factor \( \sin (\Delta \varepsilon \varepsilon_t/\hbar) / \Delta \varepsilon \) is treated as an emergent \( \delta \)-function.
When $\omega t/h \geq L_1$, then there will be few pairs of states with $\Delta E_{k,q} \in [\varepsilon_F - \hbar t^{-1}, \varepsilon_F + \hbar t^{-1}]$, and we can no longer threat $\sin(\Delta \varepsilon t/\hbar)$ as a $\delta$-function. When this happens, we start observing recurrences in the current as reported in Sec. (IV).

In this work, we investigated how a quasi-steady-state particle transport regime emerges across disordered samples coupled to large, but finite leads which are subjected to a potential bias. In order to do so, we have studied time-dependent transport, both numerically and semi-analytically, in a non-interacting and one-dimensional tight-binding chain, with open boundary conditions, where the central region is an extended disordered sample, and the rest of the chain acts as a pair of finite, but otherwise perfect leads.

For large lead size, and sufficiently large bias, a quasi-steady-state regime emerges at intermediate times, after the transient behavior has died out and before inversions in the current are observed. The current in the quasi-steady-state is approximately constant in time and homogeneous in space (if measure at points far away from the chain’s extremities). Furthermore, the value of the current in the quasi-steady-state coincides with the one predicted by the Landauer formula for semi-infinite leads, independently of the initial condition of the system (partitioned or partition-free). These results constitute an exemplification and extension to finite systems of the results of Stefanucci et al. on the establishment of a steady-state regime of transport in samples which are attached to infinite leads.

We have found that the quasi-steady-state is established, for both initial conditions, after a stabilization time $t_{\text{stab}} \approx 2v_F^{-1}L_1$. Physically, this can be interpreted as the time taken by a Fermi-level state to probe the disordered landscape inside the central sample. The quasi-steady-state lasts until a recurrence time $t_r \approx 2v_F^{-1}L_1$, where current inversions start happening. Besides being related to the inverse spacing of the energy levels in the system, this recurrence time may also be interpreted as the time taken by a Fermi-level electron to leave the sample and return to it, by traveling back and forth inside a lead. This conclusion was seen to be independent of the central sample’s features, as long as the leads are much larger than it.

During the quasi-steady-state, persistent finite-size effects are observed in the partition-free approach as superposed oscillations, with a period that is inversely proportional to the bias $\Delta V$, and an amplitude which scales to zero as $L_1 \to \infty$ but becomes more relevant (relative to $I_{\text{Landauer}}$) for very small values of $\Delta V$. This effect prevents the onset of a quasi-steady-state regime for a system prepared in the partition-free setup, if the leads are too small. In the partitioned case, the amplitude of the oscillations superposed on the quasi-steady-state plateaus is not influenced by the size of leads, but instead are damped as the observation time is increased (while keeping $t < t_r$). Similarly to the partition-free case, the amplitude of the fluctuations increases for smaller biases. These observations seem to indicate that the observation of a clear quasi-steady-state requires some kind of mechanism which scatters the electron’s momenta.

These observations constitute an exemplification and extension to finite systems of the results of Stefanucci et al. Here it is provided by the applied potential ramp in the sample, which becomes less effective mechanism as $\Delta V \to 0$. In both cases, these finite-size oscillations can be made arbitrarily small if $L_1$ is large enough.

In order to shine light on the numerical results, a time-dependent Kubo formula for the current in the partition-free approach, which is suitable for semi-analytical treatment, was developed in order to describe the local time-dependent current due to a small applied bias. From this formula, it was possible to see that an approximately time-independent and spatially uniform current emerges in the limit of large system’s size and observation times, $L_1, t \to \infty$, provided $t \ll v_F^{-1}L_1$ in agreement with the recurrence time observed numerically. These conditions are necessary to treat the leads as being effectively infinite, in what respects DC-transport. After expressing the eigenfunctions of the disordered central sample in

VI. CONCLUSIONS

Figure 10. Plots of the full prefactors $\mathcal{P}(\varepsilon_F, k - q)$ for different central samples at half-filling (upper panels) and different Fermi energies, $\varepsilon_F$ (lower panels). The collapse of all the data into the red dashed curves justifies the validity of expression of Eq. (51) for states close to the Fermi level. In both panels $\mathcal{P}_{k,q}$ is measured in units of $\omega^2/h$. (color online)
terms of complex reflection and transmission coefficients, all the matrix elements appearing in the Kubo formula were evaluated semi-analytically. The quasi-steady-state current thus obtained was shown to reproduce the Landauer formula for the current in a two-terminal device.

We hope that these theoretical predictions of the time scales over which the quasi-steady-state occurs and the nature of the finite-size oscillations can be experimentally tested and guide future research on mesoscopic transport in fermionic ultra-cold atomic gases in optical lattices.

VII. ACKNOWLEDGMENTS

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Appendix A: Review of the recursive Chebyshev method for quantum time-evolution

In this appendix, we wish to describe shortly the algorithm used to time-evolve an arbitrary single-particle state with the full Hamiltonian. As referred in the main text, the Hamiltonian generating the time-evolution for positive times, $H(t > 0)$, is time-independent and, consequently, the time-evolution operator $U_t$ reads

$$U_t = e^{-iH(t>0) t/\hbar}. \quad (A1)$$

The method used to calculate $U_t$ for our systems is based on its exact expansion as a series of Chebyshev polynomials in $H(t > 0)$, due to Tal-Ezer et al.$^{28}$ Namely, one has

$$U_t = \sum_{n=0}^{\infty} \frac{2}{1 + 2 \delta_{n,0}} (-i)^n J_n(\lambda t) T_n(\tilde{H}), \quad (A2)$$

where $\tilde{H} = \left(\frac{1}{\lambda \hbar} \right) H$ is a dimensionless Hamiltonian, rescaled by a real parameter $\lambda$ which guarantees that its spectrum is contained inside the interval $[−1, 1]$. $T_n$ is the $n$th-order Chebyshev polynomial of the first-kind, $J_n(y)$ is a Bessel function of the first kind and $t$ is a time measured in units of $\hbar$. The key to the method is to avoid the numerical diagonalization of $H(t > 0)$, and instead use the recursion relation for the Chebyshev polynomials,

$$T_{n+1}(x) = x T_n(x) - T_{n-1}(x), \quad (A3)$$

in order to evaluate all the needed $T_n(\tilde{H})$, recursively. For a generic review on the application of Chebyshev spectral method to physical problems see Ref.$^{34}$ and references within.

![Figure 11. Comparison between the exact graph for $f(x) = \text{Re} \left[ e^{ix^2} \right]$ and successive truncated Chebyshev series with the first $M = 20, 40$ and $60$ polynomials. The colored arrows stand on the values for which the corresponding approximations starts to fail. The imaginary part has an analogous behavior. (color online)](image)

Furthermore, the Chebyshev series of Eq. $\text{(A2)}$ is known to converge rather quickly, meaning that a truncated summation with $M$ terms is usually enough to describe correctly $U_t$, provided $M > t \lambda$. This convergence is illustrated in Fig. 11 and in all our calculations, we used $M = 8t\lambda$.

Notice that, in order to evaluate the current, we only require to time-evolve a given single-particle state $|\Psi\rangle$. Therefore, we do need the full matrix form of $U_t$, but instead how it acts on an arbitrary state $|\Psi\rangle$. From the expansion of Eq. $(A2)$, we know that action to be

$$|\Psi^M(t)\rangle = \sum_{n=0}^{M} \frac{2}{1 + 2 \delta_{n,0}} (-i)^n J_n(\lambda t) |\Psi_n\rangle, \quad (A4)$$

where $|\Psi_n\rangle = T_n(\tilde{H}) |\Psi\rangle$ and $M$ is the truncation order of the Chebyshev expansion.$^{35}$ Finally, the first two $|\Psi_n\rangle$ can be directly calculated by the simple forms of $T_0(x)$ and $T_1(x)$, i.e.

$$|\Psi_0\rangle = T_0(\tilde{H}) |\Psi\rangle = |\Psi\rangle \quad (A5a)$$

$$|\Psi_1\rangle = T_1(\tilde{H}) |\Psi\rangle = \tilde{H} |\Psi\rangle, \quad (A5b)$$

and then the remaining are efficiently calculated by using the operator generalization of the Chebyshev recursion [Eq. $(A3)$], i.e.

$$|\Psi_{n+1}\rangle = \tilde{H} |\Psi_n\rangle - |\Psi_{n-1}\rangle. \quad (A6)$$
Appendix B: Review of the recursive transfer matrix method

In this Appendix, we explore a very simple algorithm which allows us to calculate the transfer matrix \( M(k) \) of any given disordered sample, when it is connected to semi-infinite leads. This method is the same used in the early papers of Andereck et al\cite{andereck1992} and Pichard\cite{pichard1974} and allows for the calculation of \( M(k) \) with an \( \sim \mathcal{O}(L_S) \) number of operations.

For these purposes, it is more useful to re-express the Hamiltonian of the central sample in a first-quantization language, i.e.

\[
H_s = \sum_{n=1}^{L_s} \varepsilon_n \left| n \right\rangle \left\langle n \right| - \sum_{n=1}^{L_s-1} \left( \left| n \right\rangle \left\langle n + 1 \right| + \left| n + 1 \right\rangle \left\langle n \right| \right),
\]

where \( \left| n \right\rangle \) are the Wannier states of the chain and \( \varepsilon_n \) is an on-site energy (in units of the hopping \( w \)). To model the connection between the finite sample to the semi-infinite leads, one has also the following boundary hopping Hamiltonian:

\[
H_a = -|0\rangle \langle 1| - |1\rangle \langle 0| - |L_s-1\rangle \langle L_s + 1| - |L_s + 1\rangle \langle L_s| .
\]

The main purpose of this method is to find the scattering states associated to a particular disorder realization. For that, one must fix the leads’ propagating states, \( |\Psi_l^L\rangle \) and \( |\Psi_r^R\rangle \), as the left and right boundary conditions for the problem. This setup is represented in Fig. 12, with the counter-propagating plane-waves in the leads being represented as arrows.

![Figure 12. Schematic representation of the setup used in the implementation of the transfer matrix method. Red dots represent the disordered scattering region. The leads are represented as the lighter red “ghost” sites on both sides. (color online)](image)

Figure 12. Schematic representation of the setup used in the implementation of the transfer matrix method. Red dots represent the disordered scattering region. The leads are represented as the lighter red “ghost” sites on both sides. (color online)

1. Hamiltonian in Real-Space and Boundary Conditions

The first step towards the definition of the present method is expanding a scattering state (with wavenumber \( k \)) in the basis of Wannier wavefunctions, i.e.

\[
|\Psi_k\rangle = \sum_n \psi_n |n\rangle ,
\]

and finally rewriting the time-independent Schrödinger equation — \( \mathcal{H}|\Psi_k\rangle = E_k |\Psi_k\rangle \) — in terms of the real-space amplitudes \( \psi_n \),

\[
E_k \psi_n = \varepsilon_n \psi_n - \psi_{n-1} - \psi_{n+1} ,
\]  

where, by definition, \( \varepsilon_n = 0 \) outside of the sample.

As shown in Fig. 12, the boundary conditions are to be set as the plane-waves defined in the Eq. (30) of the main text. Reminding, one has

\[
|\Psi^L_k\rangle = \sum_{n=-L_1}^{1} \left[ \psi^L_n e^{ik(n-1)} |n\rangle + \psi^R_n e^{-ik(n-1)} |n\rangle \right] ,
\]

\[
|\Psi^R_k\rangle = \sum_{n=1}^{L_1} \left[ \psi^R_n e^{ik(n-L_2)} |n\rangle + \psi^L_n e^{-ik(n-L_2)} |n\rangle \right] .
\]

These states immediately set the amplitudes on the “ghost” sites of Fig. 12 to the following values:

\[
\psi_{-1} = \psi^L_0 e^{-2ik} + \psi^R_0 e^{2ik} ,
\]

\[
\psi_0 = \psi^L_0 e^{-ik} + \psi^R_0 e^{ik} ,
\]

\[
\psi_{L_2 + 1} = \psi^R_0 e^{ik} + \psi^L_0 e^{-ik} ,
\]

\[
\psi_{L_2 + 2} = \psi^R_0 e^{2ik} + \psi^L_0 e^{-2ik} .
\]

2. Review of the Transfer Matrix Recursion Method

Despite not having the look of a linear algebra problem, Eq. (B4) may be turned into a matrix recursion equation, when supplemented by the trivial condition

\[
\psi_n = \psi_n .
\]

Hence, we have

\[
\begin{pmatrix}
\psi_{n+1} \\
\psi_n \\
\end{pmatrix} =
\begin{pmatrix}
\varepsilon_n - E_k & -1 \\
1 & 0 \\
\end{pmatrix}
\begin{pmatrix}
\psi_n \\
\psi_{n-1} \\
\end{pmatrix} .
\]

If we now iterate Eq. (B8), we get the following relation

\[
\begin{pmatrix}
\psi_{L_2 + 2} \\
\psi_{L_2 + 1} \\
\end{pmatrix} = T_{L_2 + 1} (k) \cdot T_{L_2} (k) \cdot \cdots \cdot T_1 (k) \cdot T_0 (k) \cdot
\begin{pmatrix}
\psi_0 \\
\psi_{-1} \\
\end{pmatrix} .
\]

In the same way, we may write the boundary conditions of Eqs. (B7), as the following matrix relations:

\[
\begin{pmatrix}
\psi_0 \\
\psi_{-1} \\
\end{pmatrix} =
\begin{pmatrix}
\psi^L_0 e^{-ik} & \psi^R_0 e^{ik} \\
\psi^R_0 e^{-2ik} & \psi^L_0 e^{2ik} \\
\end{pmatrix}
\begin{pmatrix}
\psi^L_k \\
\psi^R_k \\
\end{pmatrix} ,
\]

and
\[
\begin{pmatrix}
\psi_{L+2} \\
\psi_{L+1}
\end{pmatrix} = \begin{pmatrix}
e^{2ik} & e^{-2ik} \\
e^{ik} & e^{-ik}
\end{pmatrix}
\begin{pmatrix}
\Psi^R \\
\Psi^R
\end{pmatrix},
\] (B11)

which can be inverted as
\[
\begin{pmatrix}
\Psi^R \\
\Psi^R
\end{pmatrix} = \mathbb{B}_R (k) \cdot \begin{pmatrix}
\psi_{L+2} \\
\psi_{L+1}
\end{pmatrix},
\] (B12)

Using Eqs. (B10) and (B12) into Eq. (B9), we get to the following final result:
\[
\begin{pmatrix}
\Psi^R \\
\Psi^R
\end{pmatrix} = \mathbb{B}_R (k) \cdot T_{L+1} (k) \cdot T_L (k) \cdot \cdots \cdot T_1 (k) \cdot T_0 (k) \cdot \mathbb{B}_L (k).
\] (B13)

and, by definition, the transfer matrix of the whole sample is written as:
\[
\mathcal{M} (k) = \mathbb{B}_R (k) \cdot T_{L+1} (k) \cdot T_L (k) \cdot \cdots \cdot T_1 (k) \cdot T_0 (k) \cdot \mathbb{B}_L (k).
\] (B14)

This last equation was the one we implemented to calculate \(\mathcal{M} (k)\) for any given disordered sample.

Appendix C: Emergence of selection rule

In this appendix, we prove the effective selection rule of Eq. (46). In order to do so, we will analyze the factor \(\sin [(k - q) L_i]\), when \(q, k\) belong to the same or different classes. More precisely, will calculate its absolute value, which can be written as

\[
|\sin [(k - q) L_i]| = \sqrt{1 - \cos [2 L_i (q - k)]}.
\]

where we summed and subtracted \(\phi (q) - \phi (k)\) in the argument of the cosine and, then, decomposed it using the rule for the cosine of a sum of angles. The main advantage of this form is that the continuous function \(\phi (k)\) depends solely in the properties of the central sample and the effect of increasing the leads is to populate more densely their domains with allowed values of \(k\). This, together with the fact that we are only interested in what happens near \(k_F\), allows us to expand it as Taylor series on \(\delta q = q - k_F\) and \(\delta k = k_F - k\):

\[
\phi (q) - \phi (k) = \frac{d\phi}{dk} \bigg|_{k_F} \delta q + \delta k + \cdots \approx \frac{d\phi}{dk} \bigg|_{k_F} (q - k),
\] (C2)

and, consequently,

\[
|\sin [(q - k) L_i]| \approx \sqrt{1 - \cos [2 L_i (q - k) + \phi (q) - \phi (k)]},
\] (C3)

where the corrections are of order \(q - k\) and disappear in the limits \(L_i \to \infty\) and \(\hbar t^{-1} \to 0\). At this point, all we must do is to decompose the cosine term in Eq. (C3) using the usual rules for the sum of angles and then resort to the quantization condition of Eq. (38) to realize that

\[
\cos [2 (L_i + 1) (q - k) + \phi (q) - \phi (k)] = \]

\[
\mp \sqrt{\left[1 - |r (q)|^2 \sin^2 (\theta (q) - \phi (q)) \right] \left[1 - |r (k)|^2 \sin^2 (\theta (k) - \phi (k)) \right] + |r (q)| |r (k)| \sin [\theta (q) - \phi (q)] \sin [\theta (k) - \phi (k)]},
\] (C4)

where the \(+ (-)\) sign stands for the case when \(q, k\) are in the same class (different classes) of states.

Finally, one can evoke the same argument as before to Taylor expand all the sample-specific functions appear in Eq. (C4) (to be clear, \(r (x), \theta (x), \phi (x)\) around \(k_F\), but noting that \(k < k_F < q\) by definition. Up to corrections irrelevant correction in the same limits, this gives rise to Eq. (46) of the main text after expanding the sin functions in powers of \(q - k\).
Appendix D: Calculation of the joint density of contributing states

In this appendix, we will proceed to calculate the joint density of contributing states (JDoCS), for both positive and negative $\Delta \varepsilon$. For positive energy differences, $\Delta \varepsilon > 0$, the JDoCS is defined, from Eq. (53), as

$$\rho(\varepsilon_F, \Delta \varepsilon) = \frac{1}{4L_l^2} \sum_{k,q}^\prime \delta(\Delta \varepsilon - \Delta \varepsilon_{k,q}). \quad (D1)$$

Which may be written in terms of the usual density of states for each class, $\sigma = \pm$, i.e.

$$\rho^{\sigma}(\varepsilon) = \frac{1}{L_l} \sum_{k^\sigma} \delta(\varepsilon - \varepsilon_{k^\sigma}), \quad (D2)$$

yielding the expression,

$$\rho(\varepsilon_F, \Delta \varepsilon) = \frac{1}{4} \int_{-\pi}^{\pi} d\varepsilon_1 \int_{-\pi}^{\pi} d\varepsilon_2 \lim_{L_s \to \infty} \left\{ \rho_{L_s}^{+} (\varepsilon_1) \rho_{L_s}^{-} (\varepsilon_2) + \rho_{L_s}^{-} (\varepsilon_1) \rho_{L_s}^{+} (\varepsilon_2) \right\} \delta(\Delta \varepsilon - \varepsilon_2 + \varepsilon_1), \quad (D3)$$

in the limit of semi-infinite leads.

$$\frac{\delta(\varepsilon - \varepsilon_{k^\sigma})}{L_l} \delta(\Delta \varepsilon - \Delta \varepsilon_{k,q}).$$

where $\rho(\varepsilon)$ is the full DoS of a clean infinite chain. In what follows, we will always assume that the expression of Eq. (D4) may be used to calculate de JDoCS in the limit of very large $L_l$. This intuition is confirmed by the plots of the DoS in Fig. 13, which were obtained numerically, for a randomly selected disordered sample, using the well-known kernel polynomial method with a Jackson kernel and a fixed number of polynomials, $M = 4096$, enough to resolve the individual energy levels in the smaller case considered (see Weiße et al. [14] for more details on the method). Consequently, one has the following expression for the JDoCS

$$\rho(\varepsilon_F, \Delta \varepsilon) = \int_{\varepsilon_F}^{\varepsilon_F + |\Delta \varepsilon|} \frac{\Theta(|\Delta \varepsilon| + \varepsilon - \varepsilon_2)}{2\pi^2 \sqrt{(4w^2 - \varepsilon_2^2)(4w^2 - (\varepsilon_2 + \Delta \varepsilon)^2)}} \frac{d\varepsilon_2}{(4w^2 - \varepsilon_2^2)} \frac{\Theta(|\Delta \varepsilon| + \varepsilon - \varepsilon_2)}{2\pi^2 \sqrt{(4w^2 - \varepsilon_2^2)(4w^2 - (\varepsilon_2 + \Delta \varepsilon)^2)}} \quad (D5)$$

where $\Theta(x)$ is the Heaviside function and $\Delta \varepsilon \geq 0$. The integral in Eq. (D5) can be done numerically and the curves are shown in Fig. 14 for different values of the Fermi energy $\varepsilon_F$. Nevertheless, we are only interested in the shape of $\rho(\varepsilon, \Delta \varepsilon)$ when $\Delta \varepsilon \approx 0$. For that, we may expand Eq. (D5) in powers of this quantity, yielding

$$\rho(\varepsilon_F, \Delta \varepsilon > 0) = \frac{\Delta \varepsilon}{2\pi^2 (4w^2 - \varepsilon_F^2)} + O[\Delta \varepsilon^2]. \quad (D6)$$

Finally, we can generalize Eq. (D6) to $\Delta \varepsilon < 0$, which is trivial since, by definition [Eq. (53)], we have $\rho(\Delta \varepsilon) = \rho(-\Delta \varepsilon)$. Hence, our final expression is simply,

$$\rho(\varepsilon_F, \Delta \varepsilon) = \frac{1}{2\pi^2 (4w^2 - \varepsilon_F^2)} + O[\Delta \varepsilon^2], \quad (D7)$$

which is the one we use in the main text [Eq. (54)].

Figure 13. Plots of the DoS calculated using the KPM for a system with leads of different sizes and a central sample without (black curve) and with disorder (colored curves). The number of Chebyshev moments used is $M = 4096$ for all the cases. The insets are zooms made to the regions indicated by the black boxes in the main graph, where one can clearly see the spectral weight of the states in the sample being out-weighted by the states coming from the finite clean leads. (color online)

To progress beyond Eq. (D3) in a general fashion, one starts by recognizing that, since $\rho^{\pm}(\varepsilon)$ is an intensive quantity. So these must be dominated by the states on the (clean) leads, as $L_l \to \infty$. Since we know that, for a clean system, the states of different parities are alternated in $k$-space, with a regular separation given by $\pi/L_l$, one concludes that

$$\lim_{L_l \to \infty} \rho_{L_l}^{\pm}(\varepsilon) = \rho(\varepsilon) = \begin{cases} \frac{1}{\pi \sqrt{4w^2 - \varepsilon^2}} & \text{if } |\varepsilon| \leq 2w \\ 0 & \text{if } |\varepsilon| > 2w \end{cases}, \quad (D4)$$

Figure 14. Plots of the JDoCS from the numerical integration of Eqs. (D5) for different values of the Fermi energy and positive values of $\Delta \varepsilon$. The dashed straight lines are plots of the linear approximations near $\varepsilon_F$, as calculated in Eq. (D6). (color online)
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