Length-dependent oscillations in the dc conductance of laser-driven quantum wires

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(Received 15 October 2007; revised manuscript received 5 May 2008; published 25 July 2008)

We calculate the dc conductance at zero temperature of clean quantum wires driven by a laser field. In the high-frequency regime we find an interplay between length-dependent interference effects and dynamical localization, which leads to a modulation by a Bessel function of the even-odd oscillations in the conductance. In the low-frequency regime we find that the field suppresses these oscillations. We present some analytical expressions for each of these frequency limits.

DOI: 10.1103/PhysRevB.78.045428 PACS number(s): 73.21.Hb, 72.10.−d, 73.23.−b

I. INTRODUCTION

Quantum wires will be the basic components in quantum electronic devices. Understanding their basic electronic transport properties is of fundamental importance for future applications. Experimentally, chains of atoms between two electrodes have been formed and investigated[1–3] and the conductance of molecules like H_2 has been measured.[4] Carbon nanotubes are also very promising materials for working as quantum wires in different possible devices.[5]

One of the most basic properties of the conductance in clean quantum wires is its oscillations as a function of the wire length.[6] When the Fermi energy E_F is located in the band center of a one-dimensional wire even-odd oscillations have been known to exist since the beginning of the field of molecular electronics.[7] They can be seen as analogous to a Fabry-Perot interferometer for electronic transport. The conductance of atomic Au, Pt, and Ir wires between break junction contacts has revealed these oscillations. For an odd number of atoms in the atomic wire the conductance has maxima while it is reduced when the number of atoms is even.[8] This behavior was obtained after averaging over many realizations of the experiment in which the precise form of the contacts between the electrodes and the atomic chain might be different. Using density functional methods these oscillations have been calculated for chains of Na atoms[9] and a four-atom period was obtained for Al atoms.[10] Depending on the value of E_F oscillations of different periods have been shown to appear.[11] These oscillations survive in the presence of interactions[12] which can increase their amplitude with the length.[11,13,14]

One interesting possibility to control the properties of a quantum wire is to use a time-dependent electromagnetic field such as that of a laser beam. Interesting phenomena have been found in the last decade, such as photon assisted tunneling,[15,16] pumping of electrons,[17–21] heat pumping,[22,23] and quantum rachet effect in molecules.[24] Theoretically, an important breakthrough was the recent derivation of a Landauer-type formula[25] for transport in driven systems using Floquet theory.[26] The current and the noise in coherent conductors connected to leads have been written in terms of transmission coefficients that could be calculated using the Floquet-Green function of the system.

It is the objective of this paper to study the dc conductance of a quantum wire modeled with a tight-binding Hamiltonian in the presence of a laser field (dipole approximation.) For that purpose we will use a Floquet-Green function formalism. The Floquet-Green function will be computed using a matrix continued fraction method[27,28] that has been successfully used for studying the localization properties of disordered one-dimensional systems.[29,30]

The remainder of the paper is organized as follows: In Sec. II the Floquet formulation of the conductance for driven systems is sketched and the method of calculation of the Floquet-Green function for our tight-binding quantum wire connected to leads is explained. The modulation of the even-odd oscillations due to dynamical localization in the high-frequency regime is studied in Sec. III where we compare our exact results using the Floquet-Green function of the system, with the analytical results obtained in the high-frequency limit. In Sec. IV we obtain analytical results within the low-frequency approximation and we compare them with the exact results. Finally, we end with some conclusions and perspectives in Sec. V. In the Appendix we have presented the derivation for the even-odd oscillations in terms of the Green's function, which establishes a connection between the driven and nondriven results.

II. FLOQUET-GREEN FORMULATION OF THE CONDUCTANCE FOR DRIVEN SYSTEMS

Following Ref. 26, we describe our laser-driven quantum wire by a time-dependent Hamiltonian of the form

$$H(t) = H_{\text{wire}}(t) + H_{\text{leads}} + H_{\text{coupling}}, \tag{1}$$

where the different terms correspond to the time-dependent Hamiltonian for the quantum wire, the Hamiltonian for the leads, which we assume as time independent, and the lead-wire coupling, respectively. We want to study the basic physics at play in the regime of coherent quantum transport in the presence of the driving field.

We will neglect the possible effects of the electron-electron interaction and the effect of dissipation in the wire. The effect of the oscillating potential in the leads could be important and modify the tunneling rates in general; see for

example Ref. 31 for a 2D case. However, for the one-dimensional models considered in this work, the effect of an oscillating external voltage applied to the leads can be mapped to the Hamiltonian in Eq. 1 by a gauge transformation; see page 387 of Ref. 26. For this reason and for simplicity we will not include any time dependence in the leads or in the couplings.

For the wire Hamiltonian we choose a tight-binding model composed of L sites with next-neighbor hopping and an oscillating dipole field that could represent a laser with an angle of incidence perpendicular to the wire and an angle of polarization parallel to the wire.

$$H_{\text{wire}}(t) = -s\sum_{l=1}^{L-1}(|l\rangle\langle l+1| + |l+1\rangle\langle l|) + 2v\cos(\omega t)\sum_{l=1}^{L} l|l\rangle\langle l|, \tag{2}$$

where s is the hopping matrix element ($4s$ corresponds to the bandwidth of the wire), ω is the frequency of the laser, and $2v$ is the amplitude of its electric field. The factor of 2 is used here for later convenience.

The leads are modeled by ideal electron gases,

$$H_{\text{leads}} = \sum_k \epsilon_k (c_{Lk}^\dagger c_{Lk} + c_{Rk}^\dagger c_{Rk}), \tag{3}$$

where $c_{L(R)k}^\dagger$ creates an electron with momentum k in the left (right) lead. The coupling between the wire and the lead is modeled by the tunneling Hamiltonian connecting the Fermi gas states of the left lead to the first site in the wire and the states of the right lead to the last site of the wire,

$$H_{\text{coupling}} = \sum_k (V_{Lk} c_{Lk}^\dagger c_1 + V_{Rk} c_{Rk}^\dagger c_L + \text{H.c.}). \tag{4}$$

The coupling matrix elements will be considered symmetric $V_{kL} = V_{kR}$. They can be described by a spectral density

$$\Gamma_{L(R)}(E) = 2\pi\sum_k |V_{L(R)}|^2 \delta(E - \epsilon_k). \tag{5}$$

We will use the wide-band limit approximation for these couplings and consider them energy independent. This approximation is justified when the conduction bandwidth of the leads is much larger than all other relevant energy scales.

In the wide-band approximation, the effect of the Hamiltonian of the leads and the coupling to the wires can be taken care of by introducing two self-energies into the Hamiltonian of the wire, the resulting operator H, which is often called an "effective Hamiltonian," is nonHermitian. For a clean wire driven by a laser field it can be written as

$$H_{\text{wire}}^{\text{eff}}(t) = H_0 + 2v\cos\omega t\sum_{l=1}^{L} l|l\rangle\langle l| + i\Gamma_L|1\rangle\langle 1| + i\Gamma_R|L\rangle\langle L|, \tag{6}$$

with H_0 defined as the tight-binding Hamiltonian (first term on the right-hand side) in Eq. (2).

In Fig. 1 we show a schematic drawing of the kind of systems that we consider in this work.

From this point on, we will refer to the operator $H_{\text{wire}}^{\text{eff}}(t)$ as our "Hamiltonian" $H(t)$, even though it is clearly a non-

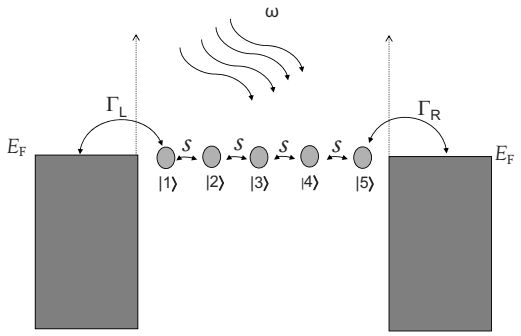

FIG. 1. Schematic representation of a quantum wire with five sites as modeled in the text.

Hermitian operator. Effective Hamiltonians of this kind have been rigorously defined and have been used for a long time to describe, for instance, the physics of decay from open systems. In the mathematical treatment that follows using the Floquet-Green operator, the nonhermicity of $H(t)$ plays no significant role and its particulars features will be pointed out only when necessary.

Since our (effective) Hamiltonian for the wire is time-periodic, $H(t) = H(t+T)$, with period $T = 2\pi/\omega$, we can apply Floquet theory.[32–34] The solutions to the Schrödinger equation $\Psi(t)$ with a Hamiltonian that is time-periodic are of the form

$$|\Psi^e(t)\rangle = e^{-iet/\hbar}|\phi^e(t)\rangle, \tag{7}$$

where $|\phi^e(t)\rangle = |\phi^e(t+T)\rangle$. One can arrive at an eigenvalue equation for the Floquet Hamiltonian $H^F(t) \equiv H(t) - i\hbar\frac{\partial}{\partial t}$,

$$H^F(t)|\phi^e(t)\rangle = e|\phi^e(t)\rangle. \tag{8}$$

As pointed out by Sambe,[34] since Eq. (8) is an eigenvalue equation, it can be solved using the standard techniques developed for time-independent Hamiltonians, provided we extend the Hilbert space of the system, $\mathcal{H}$, to include the space of time-periodic functions. If $e_{\alpha,p}$ is an eigenvalue with corresponding eigenvector $|\phi^{e_{\alpha,p}}(t)\rangle$, then $e_{\alpha,p} + m\hbar\omega$ is also an eigenvalue with corresponding eigenvector $|\phi^{e_{\alpha,p}+m\hbar\omega}(t)\rangle = e^{im\omega t}|\phi^{e_{\alpha,p}}(t)\rangle$. Accordingly, the eigenstate corresponding to the eigenvalue $e_\alpha + m\hbar\omega$ has the same structure as the eigenstate corresponding to $e_{\alpha,p}$, except that it is displaced by $m\hbar\omega$ on the energy axis. Because of this, to find all the eigenvectors and eigenvalues of the Floquet Hamiltonian one needs only to consider $-\frac{1}{2}\hbar\omega \le \text{Re}(e) < \frac{1}{2}\hbar\omega$. We use the letter ϵ to refer to the Floquet eigenvalues restricted to this interval and call them, as it is customary, "quasi-energies." For the particular case of our operator $H_{\text{wire}}^{\text{eff}}(t)$, the quasi-energies are complex, with $\text{Im}(\epsilon_\alpha)$ (often called "self-energy") being dependent on the couplings $\Gamma_{R/L}$ to the leads.

The Floquet-Green operator corresponding to Eq. (8) is defined by (see Refs. 27 and 28)

$$[\mathbb{I}E - H^F(t')]G(E,t',t'') = \mathbb{I}\delta_\tau(t'-t''), \tag{9}$$

where $\delta_\tau(t)$ is the τ-periodic delta function ($\tau = \frac{2\pi}{\omega}$) and $\mathbb{I}$ is the identity operator in $\mathcal{H}$. We can write the Floquet-Green operator entirely in terms of the eigenfunctions $|\phi^{\alpha,0}(t)\rangle$,

which correspond to values $e_{\alpha,p}$ where $-\frac{1}{2}\hbar\omega < \mathrm{Re}(e_{\alpha,p}) < \frac{1}{2}\hbar\omega$.

$$G(E,t',t'') = \sum_{\alpha}\sum_{p} e^{ip\omega(t'-t'')}\frac{|\phi^{\alpha,0}(t')\rangle\langle\phi^{\alpha,0}(t'')|}{E-\epsilon_{\alpha}-p\hbar\omega}, \quad (10)$$

where $\alpha=1,\ldots,N$ for a N-dimensional $\mathcal{H}$, and $p=-\infty,\ldots,\infty$.

Operating on both sides of this equation with $\frac{1}{\tau^2}\int_0^\tau\int_0^\tau e^{im\omega t'}e^{-in\omega t''}dt''dt'$ we can write the Floquet-Green function in terms of its Fourier components,

$$G^{m,n}(E) = \sum_{\alpha,p}\frac{1}{E-\epsilon_{\alpha}-p\hbar\omega}|\phi^{\alpha,0}_{m+p}\rangle\langle\phi^{\alpha,0}_{n+p}|, \quad (11)$$

where

$$G^{m,n}(E) = \frac{1}{\tau^2}\int_0^\tau\int_0^\tau e^{im\omega t'}e^{-in\omega t''}G(E,t',t'')dt''dt',$$

and

$$|\phi^{\alpha,0}_{m}\rangle = \frac{1}{\tau}\int_0^\tau e^{im\omega t'}|\phi^{\alpha,0}(t')\rangle dt', \quad (12)$$

$m,n=-\infty,\ldots,\infty$. It is easy to show that the components of the Floquet-Green function have the following property: $G^{m,n}(E)=G^{m-k,n-k}(E+k\hbar\omega)$. From this one can conclude that the quantities $G^{k,0}(E)$ provide all the information of the driven system, and from now on we will call them $G^{(k)}(E)$.

$$G^{(k)}(E) = \sum_{\alpha,p}\frac{1}{E-\epsilon_{\alpha}-p\hbar\omega}|\phi^{\alpha,0}_{k+p}\rangle\langle\phi^{\alpha,0}_{p}|. \quad (13)$$

In our case, $H^{\mathrm{eff}}_{\mathrm{wire}}(t)$ is nonHermitian, and therefore $|\phi^{\alpha,0}_{k+p}\rangle$ and $\langle\phi^{\alpha,0}_{p}|$ are, correspondingly, a right eigenvector and a left eigenvector of the Floquet Hamiltonian $(H^{\mathrm{eff}}_{\mathrm{wire}})^F$.

The physical interpretation of the operators $G^{(k)}(E)$ above is simple. They give the probability amplitude for the propagation of a particle with initial energy E to a final energy $E+k\hbar\omega$ having absorbed or emitted $|k|$ photons (for k being positive or negative, respectively).

For one-dimensional systems, in the case of the wide-band limit previously considered, we can write the average current through the driven system in terms of the Floquet-Green operators $G^{(k)}(E)$ corresponding to the effective wire Hamiltonian,[26]

$$\bar{I} = \frac{e}{h}\sum_{k=-\infty}^{\infty}\int dE[T^{(k)}_{LR}(E)f_R(E) - T^{(k)}_{RL}(E)f_L(E)], \quad (14)$$

with

$$T^{(k)}_{LR}(E) = \Gamma_R\Gamma_L|G^{(k)}_{1L}(E)|^2,$$

$$T^{(k)}_{LR}(E) = \Gamma_R\Gamma_L|G^{(k)}_{1L}(E)|^2, \quad (15)$$

and $f_{L(R)}(E)$ being the Fermi functions corresponding to the left and right lead. $\Gamma_{L(R)}$ represent the coupling to the left (right) lead, as defined in Eq. (5), and the subscripts in the Green's function relate to the matrix elements of $G^{(k)}$ between the first site of the system connected to the left lead and the last site of the system of length L, connected to the right lead.

If we define the dc conductance at zero temperature as

$$g = \lim_{V\to 0}\frac{d\bar{I}}{dV}, \quad (16)$$

where V is the applied bias between the leads that will modify the Fermi factors corresponding to the right and left leads, we can easily arrive at a formula for the conductance at $T=0$ for one-dimensional driven systems,

$$g = \frac{e}{2h}[\tilde{T}_{LR}(E_F) + \tilde{T}_{RL}(E_F)], \quad (17)$$

where

$$\tilde{T}_{LR(RL)}(E_F) \equiv \sum_{k=-\infty}^{\infty} T^{(k)}_{LR(RL)}(E_F). \quad (18)$$

If the system *does not* have a reflection symmetry $T^{(k)}_{LR}(E)$ is not necessarily equal to $T^{(k)}_{RL}(E)$. In our case, however, the nondriven part of the Hamiltonian in Eq. (2) is spatially symmetric, and therefore one can prove that $T^{(k)}_{LR}(E)=T^{(k)}_{RL}(E)$ and therefore $\tilde{T}_{LR}(E)=\tilde{T}_{RL}(E)=\tilde{T}(E)$. [This implies that there is no pumped current in our system, since $\bar{I}=0$ when $V=0$, as can be seen from Eq. (14)]. Using this we obtain

$$g = \frac{e}{h}\tilde{T}(E_F). \quad (19)$$

Equation (19) is the basic formula that we use throughout this paper.

In order to calculate the Floquet-Green function Fourier components we use the matrix continued fractions formalism as presented in Ref. 27. Here we will only write down the final expressions for a general Hamiltonian of the form $H=H_{\mathrm{static}}+2V\cos(\omega t)$, where H_{static} and V are time-independent operators in the Hilbert space of the system.

$$G^{(0)}(E) = [E - H_{\mathrm{static}} - V_{\mathrm{eff}}(E)]^{-1}, \quad (20)$$

where

$$V_{\mathrm{eff}} = V^{+}_{\mathrm{eff}}(E) + V^{-}_{\mathrm{eff}}(E),$$

with

$$V^{\pm}_{\mathrm{eff}}(E) = V\cfrac{1}{E\pm 1\hbar\omega - H_0 - V\cfrac{1}{E\pm 2\hbar\omega - H_0 - V\cfrac{1}{\ddots}V}}V, \quad (21)$$

and

$$G^{(k)}(E) = \prod_{j=0}^{j=|k|-1} V^{-1}V^{sg(k)}_{\mathrm{eff}}(E + sg(k)j\hbar\omega)G^{(0)}(E), \quad (22)$$

where $sg(k)=+(-)$ for $k>0(k<0)$. For details about this method we refer the reader to the original references.[27,28]

This is the method that we will use to calculate *exactly* the

conductance in the following sections. Using Eqs. (20)–(22) we calculate numerically the Floquet-Green function of the effective Hamiltonian $H_{\text{wire}}^{\text{eff}}$, where $H_{\text{static}}=H_0+i\Gamma_L|1\rangle\langle 1|+i\Gamma_R|L\rangle\langle L|$ and $V=v\Sigma_{l=1}^{L}l|l\rangle\langle l|$. The matrix elements of the Green's function calculated in this way will be introduced in Eq. (14) to compute the current, from which one can obtain the dc conductance g. The results of these calculations will be labeled "exact" in the figures of the sections to come.

III. MODULATION OF THE EVEN-ODD OSCILLATIONS IN THE HIGH-FREQUENCY REGIME

Using the effective Hamiltonian for the wire we can obtain the time evolution for the part of the wave function that remains in the wire after a time t, $\varphi_l(t)$. It satisfies

$$i\hbar\frac{d}{dt}\varphi_l(t)=[H_0+2v\cos\omega t l+i\Gamma_L\delta_{l1}+i\Gamma_R\delta_{lL}]\varphi_l(t), \tag{23}$$

where $\varphi_l(t)=\langle l|\varphi(t)\rangle$, for $l=1,\ldots,L$.

If we now write $\varphi_l(t)=e^{-i2v/\hbar\omega l\sin\omega t}\psi_l(t)$ we get

$$i\hbar\frac{d}{dt}\psi_l(t)=(-se^{-i\nu\sin\omega t}\mathbb{P}^{+}-se^{i\nu\sin\omega t}\mathbb{P}^{-}+i\Gamma_L\mathbb{P}_1+i\Gamma_R\mathbb{P}_L)\psi_l(t), \tag{24}$$

where we have defined the operators $\mathbb{P}_l\equiv|l\rangle\langle l|$ and $\mathbb{P}^{+}\equiv\Sigma_{l=1}^{l-1}|l+1\rangle\langle l|$, $\mathbb{P}^{-}\equiv\Sigma_{l=2}^{L}|l-1\rangle\langle l|$ and the dimensionless quantity $\nu=2v/\hbar\omega$.

A dimensionalizing the equation above, using $\Theta=\omega t$ we obtain

$$i\frac{d}{d\Theta}\psi_l(\Theta)=H(\Theta)\psi_l(\Theta), \tag{25}$$

with

$$H(\Theta)=-\frac{s}{\hbar\omega}e^{-i\nu\sin\Theta}\mathbb{P}^{+}-\frac{s}{\hbar\omega}e^{i\nu\sin\Theta}\mathbb{P}^{-}+i\frac{\Gamma_L}{\hbar\omega}\mathbb{P}_1+i\frac{\Gamma_R}{\hbar\omega}\mathbb{P}_L. \tag{26}$$

In the high-frequency limit, the hopping matrix element s and the coupling to the leads Γ_L,Γ_R are all small compared to $\hbar\omega$, which gives $H(\Theta)\ll 1$. From this one can conclude that the evolution operator corresponding to $H(t)$ should be well approximated by using first-order time-dependent perturbation theory,

$$U(t,0)=\mathbb{I}-\frac{i}{\hbar}\int_0^t H(t')dt'+\sigma(H^2). \tag{27}$$

Using the property

$$e^{ix\sin\omega t'}=\sum_{n=-\infty}^{\infty}e^{in\omega t'}J_n(x), \tag{28}$$

one obtains

$$\frac{i}{\hbar}\int_0^t H(t')dt'=-i\frac{s}{\hbar}\mathbb{P}^{+}\left[J_0(-\nu)t+\sum_{n\neq 0}\frac{e^{in\omega t}-1}{in\omega}J_n(-\nu)\right]-i\frac{s}{\hbar}\mathbb{P}^{-}\left[J_0(\nu)t+\sum_{n\neq 0}\frac{e^{in\omega t}-1}{in\omega}J_n(\nu)\right]-\frac{1}{\hbar}\Gamma_L\mathbb{P}^{1}t-\frac{1}{\hbar}\Gamma_R\mathbb{P}^{L}t, \tag{29}$$

and since in the high-frequency regime $\frac{s}{\hbar\omega}\ll 1$,

$$\frac{i}{\hbar}\int_0^t H(t')dt'\approx\frac{i}{\hbar}J_0(\nu)H_0t-\frac{1}{\hbar}\Gamma_L\mathbb{P}^{1}t-\frac{1}{\hbar}\Gamma_R\mathbb{P}^{L}t+\sigma\left(\frac{s}{\hbar\omega}\right). \tag{30}$$

This equation shows that for high frequencies, the solutions $\psi_l(t)$ of Eq. (24) can be written as $\psi_l^n(t)=e^{-iE_nt}\eta_l^n$, with η_l^n being the (right) eigenfunctions of a time-independent effective Hamiltonian

$$H'=J_0(\nu)H_0+i[\Gamma_L\mathbb{P}_1+\Gamma_R\mathbb{P}_L], \tag{31}$$

with E_n as the corresponding (complex) eigenvalues.

Since $|\varphi^n(t)\rangle=e^{-iE_nt}e^{-i\nu l\sin\omega t}|\eta^n\rangle$, the Fourier components of the Floquet eigenstates corresponding to Eq. (23) can be written as

$$|\phi_k^n\rangle=\sum_l|l\rangle J_k(-\nu l)\langle l|\eta^n\rangle. \tag{32}$$

Inserting this result into the Floquet-Green operator of the full Hamiltonian, Eq. (13), one obtains

$$G_{1L}^{(k)}(0)=J_k(-\nu)J_0(\nu L)\sum_n\frac{\langle 1|\eta^n\rangle\langle\eta^n|L\rangle}{-E_n}=J_k(-\nu)J_0(\nu L)G'_{1L}(0), \tag{33}$$

where E_n are the complex eigenvalues of the Hamiltonian H' in Eq. (31), and $G'(E)$ is the corresponding Green's function. The quantity $G'_{1L}(0)$ can be obtained directly from Eq. (A9) by replacing $s\to sJ_0(\nu)$. With this we obtain

$$G_{1L}^{(k)}(0)=J_k(-\nu)J_0(\nu L)\begin{cases}\dfrac{sJ_0(\nu)(-1)^{L/2+1}}{s^2J_0^2(\nu)+\Gamma_L\Gamma_R}, & L\ \text{even}\\ \dfrac{i}{\Gamma_L+\Gamma_R}(-1)^{L-1/2}, & L\ \text{odd}.\end{cases} \tag{34}$$

The transmission is $\tilde{T}_{LR}=\Sigma_{k=-\infty}^{\infty}\Gamma_L\Gamma_R|G_{1L}^{(k)}(0)|^2$, and from the property of Bessel functions $\Sigma_{k=-\infty}^{\infty}J_k^2(x)=1$ we finally arrive at

$$g=4\Gamma_L\Gamma_RJ_0^2(\nu L)\begin{cases}\dfrac{s^2J_0^2(\nu)}{(s^2J_0^2(\nu)+\Gamma_L\Gamma_R)^2}, & L\ \text{even}\\ \dfrac{1}{(\Gamma_L+\Gamma_R)^2}, & L\ \text{odd}.\end{cases} \tag{35}$$

Notice that due to the Bessel function factors that appear in the conductance, the amplitude of the driving field can substantially affect the conductance of these devices, and in

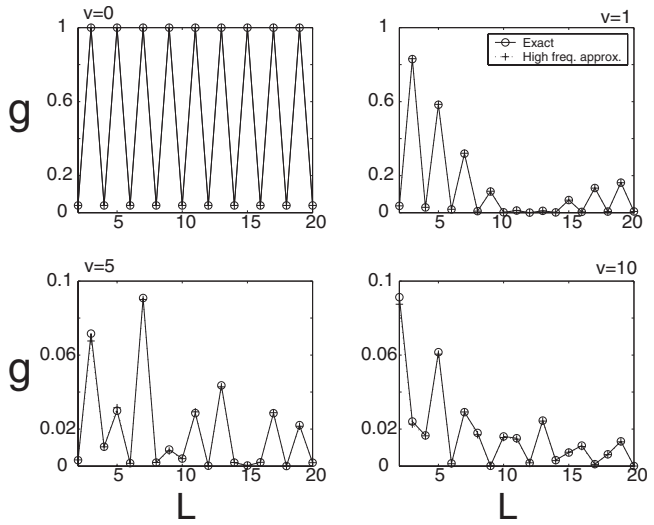

FIG. 2. Dc conductance g, as a function of the length of the wire for hopping matrix element $s=1$, coupling to the leads given by $\Gamma=0.1$, laser frequency $\omega=10$, and for different values of the field amplitude v.

fact, at some particular values, conductance can be greatly reduced (dynamic localization phenomenon). For the odd case it is interesting to notice the absence of the factor $J_0(\nu)$ in the equation above. This stems from the somewhat counterintuitive fact that for the nondriven system the conductance, for L odd, is independent of the coupling s between sites (see note at the end of the Appendix). Due to this, the phenomenon of dynamic localization, extensively discussed in the literature since it was first reported by Dunlap and Kenkre,[35] manifests itself in different ways for even and odd number of sites. In the former case the conductance is greatly reduced at values of the amplitude of the driving field v which satisfy $\nu=2v/\hbar\omega=a_{n,0}$, where $J_0(a_{n,0})=0$, and also, for $\nu=a_{n,0}/L$. In the odd case, however, only the last condition, which is length-dependent, applies. In the high-frequency regime the conductance should decrease substantially at the dynamic localization points $\nu=a_{n,0}$ without actually vanishing completely, a consequence of the fact that in deriving Eq. (35) we neglected second-order terms in $s/\hbar\omega$ which would be dominant when $J_0(\nu)$ vanishes. It is not the purpose of this work to study in detail dynamic localization and therefore, we do not include here any results for the case $\nu=a_{n,0}$.

Figure 2 shows the results for hopping matrix element $s=1$, coupling to leads $\Gamma=0.1$, laser frequency $\omega=10$, and for different values of the laser field amplitude v. For $v=0$ one can see the well-known oscillations in the conductance for L even-odd. As the laser is turned on (v increases), these oscillations become quite irregular and the conductance in general decreases with an irregular oscillatory behavior. For $\omega=10$, we can see that the agreement between the exact calculations and the high-frequency approximation is very good.

In Fig. 3 we look at the behavior of the conductance vs the length of the wire for different frequencies and for the parameters $s=1$, $\Gamma=1$, and $v=5$ (no oscillations in this case for the nondriven Hamiltonian). From these plots it is clear

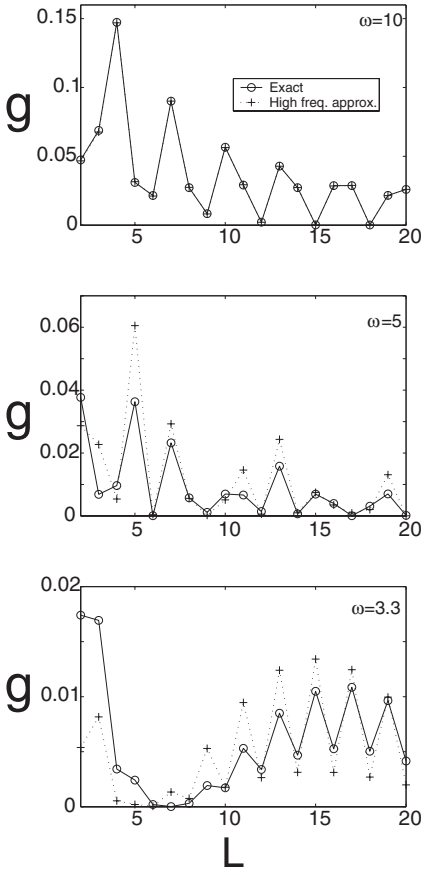

FIG. 3. Dc conductance as a function of the length of the wire for $s=1$, $\Gamma=1$, $v=5$ and three different frequencies of the driving field.

that the high-frequency regime sets in when $\frac{\Gamma}{\hbar\omega}, \frac{s}{\hbar\omega} \lesssim 0.1$. This regime is reached independently of the particular value of L, which as we will see next, is not the case for the low-frequency regime in which the convergence to the low-frequency limit is dependent on the particular length of the system. Notice that the driving induces its own oscillations in the conductance, as expected from Eq. (35) above, given the dependence of J_0 on L. These oscillations are superimposed on the oscillations that are already present in the nondriven Hamiltonian when $s \neq \Gamma$.

IV. LOW-FREQUENCY REGIME AND THE ADIABATIC LIMIT

Moskalets and Büttiker[36] have shown that when the driving frequency is much smaller than any of the energy scales of the Hamiltonian, the Floquet-Green operator of the system can be obtained from the Green operator of the stationary Hamiltonian in the following way:

$$G^{(k)}_{\text{adiab}}(E) = \frac{1}{T}\int_0^T e^{ik\omega t} G^{\text{st}}(E, v\cos\omega t)dt, \tag{36}$$

where $G^{\text{st}}(E,v)$ corresponds, in our case, to the Green's function of a tight-binding Hamiltonian with a static electric field of magnitude v.

To study this adiabatic limit we would like to compare the exact numerical results using matrix-continued fractions with Eq. (36). The diagonal elements of the Green's function for a finite 1D tight-binding system with a static electric field and *not* connected to any leads ($\Gamma=0$) have already been calculated.[37] In that work, the authors derived continued fraction expressions for the diagonal elements of the Green's function and used the properties of continued fractions to express their results in terms of ratios of Bessel functions. Using this approach we calculate analytically the Green's function of the tight-binding Hamiltonian with a static electric field and connected to the leads. First we show the results for the matrix elements G_{11}, G_{LL} and G_{1L} for the uncoupled case $\Gamma=0$, and then, using Dyson's equation, we derive the general result for $\Gamma\neq 0$. We use in Eq. (36) the analytical result thus obtained and compare it with the exact numerical result.

The Hamiltonian for a 1D tight-binding Hamiltonian with a static electric field is

$$H = H_0 + v\sum_{l=1}^{L} l|l\rangle\langle l|, \tag{37}$$

with H_0 as described in Eq. (A2). Following Ref. 37 one obtains

$$G_{11}(0,v) = \frac{1}{s}\frac{J_{L+1}(x)Y_1(x) - J_1(x)Y_{L+1}(x)}{J_0(x)Y_{L+1}(x) - J_{L+1}(x)Y_0(x)},$$

$$G_{LL}(0,v) = -\frac{1}{s}\frac{J_0(x)Y_L(x) - J_L(x)Y_0(x)}{J_0(x)Y_{L+1}(x) - J_{L+1}(x)Y_0(x)},$$

$$G_{1L}(0,v) = -\frac{1}{s}\frac{J_0(x)Y_1(x) - J_1(x)Y_0(x)}{J_0(x)Y_{L+1}(x) - J_{L+1}(x)Y_0(x)}, \tag{38}$$

with $x\equiv 2s/v$, $Y_L(x)$ are the Bessel functions of the second kind of order L, and there is no coupling to the reservoirs.

To include the effect of a coupling to the reservoirs of the form $V=i\Gamma_L|1\rangle\langle 1|+i\Gamma_R|L\rangle\langle L|$, we proceed as before, using Dyson's equation for $H=H_0+v\Sigma_{l=1}^{L} l|l\rangle\langle l|$ and V.

$$G = G^0 + G^0VG. \tag{39}$$

From Eq. (A8), with $\Gamma_L=\Gamma_R=\Gamma$, and using Eq. (38), we get

$$\begin{aligned} G_{1L}^{\mathrm{st}}(0,v) = &-s(J_0Y_{L+1} - J_{L+1}Y_0)(J_0Y_1 - J_1Y_0) \\ &\times\{s^2(J_0Y_{L+1} - J_{L+1}Y_0)^2 \\ &- is\Gamma(J_{L+1}Y_1 + J_LY_0 - J_1Y_{L+1} - J_0Y_L) \\ &\times(J_0Y_{L+1} - J_{L+1}Y_0) - \Gamma^2[(J_{L+1}Y_1 - J_1Y_{L+1})(J_0Y_L \\ &- J_LY_0) - (J_0Y_1 - J_1Y_0)^2]\}^{-1}, \end{aligned} \tag{40}$$

with all the Bessel functions evaluated at $x=2s/v$. This equation is the general expression for the Green operator component G_{1L} of a tight-binding Hamiltonian with a constant electric field and connected to leads. From it, the conductance through this system can be obtained directly. As far as we know this result has not been derived before.

In Fig. 4 we show the results for the conductance, with hopping matrix element $s=1$, coupling to leads $\Gamma=1$, laser amplitude $v=0.1$, and for different values of the laser frequency. The results were obtained by evaluating $G_{1L}^{\mathrm{st}}(0,v)$ in the above expression, replacing $v\to 2v\cos\omega t$, and using Eq. (36), together with

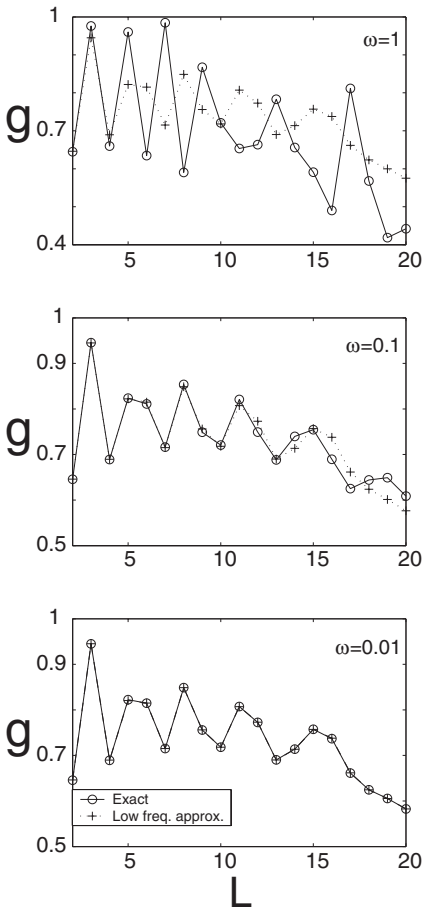

FIG. 4. Dc conductance g as a function of the length of the wire for $\Gamma=1$, $s=2$, $v=0.1$ and for different frequencies.

$$g = 4\Gamma^2\sum_{k=-\infty}^{\infty}|G_{1L}^{(k)}|^2. \tag{41}$$

We can see in Fig. 4 that the adiabatic approximation works better for lower frequencies and for the smaller lengths L. The general criteria is, according to Ref. 36, $n_{\max}\hbar\omega \ll \delta E$, where $n_{\max}$ is the maximum number of Floquet sidebands necessary to obtain convergence and δE is the minimum energy scale over which the Green's function varies significantly. For small L, typically $\delta E\approx\Gamma$ and for large L, when resonances overlap, $\delta E\approx 4s$. For an ac electric field, the number of Floquet sidebands increases linearly with L, which means that the bigger values of L require smaller frequencies to achieve convergence to the adiabatic limit, as can be observed in Figs. 4 and 5.

Notice that there are two differences between Figs. 4 and 5. The first one is that the ratio between s and Γ in Fig. 4 gives odd-even oscillations for the nondriven case ($v=0$), whereas in Fig. 5 it does not. The second difference is that in the former figure, the amplitude of the laser field is weak, whereas in the latter one it is stronger. Comparing these two

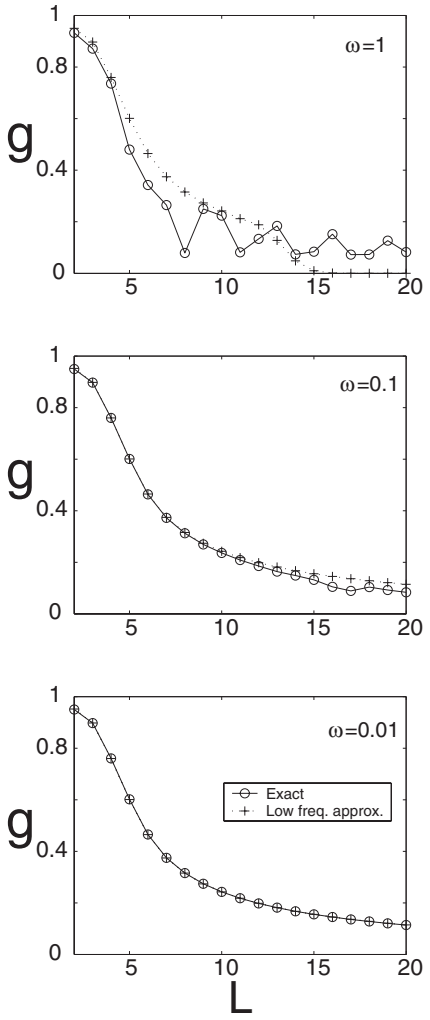

FIG. 5. Dc conductance g as a function of the length of the wire for $\Gamma=2$, $s=2$, $v=0.5$ and for different frequencies.

figures, and taking into account these differences we conclude that the even-odd oscillatory behavior of the nondriven system, in the adiabatic limit, is only preserved in a limited range of L, beyond which the localizing behavior of a quasistatic electric field (Wannier-Stark effect) dominates and the conductance decreases monotonically with L. This decay is faster for stronger field amplitudes. In the case where there are no oscillations in the nondriven conductance, as in Fig. 5, a low-frequency field does not induce any oscillations in the conductance. To summarize, a low-frequency field tends to suppress the conductance oscillations and overall decreases conductance for the longer systems.

In Fig. 6 we show different $g(L)$ curves to illustrate the fact that by manipulating the frequency and amplitude of a laser field the conductance of a quantum wire can be set to almost any value between 0 and 1 which could have interesting applications for optical switching.

In a realistic wire molecule, the hopping matrix element s is of the order of 0.1 eV with a typical wire-lead hopping rate $\Gamma=0.1s$. This is smaller than the bandwidth of the connecting leads (≈ 1 eV), which justifies the use of the wide-band approximation (Γ energy independent). To explore the high-frequency regime a frequency $\hbar\omega=10s=1$ eV could be

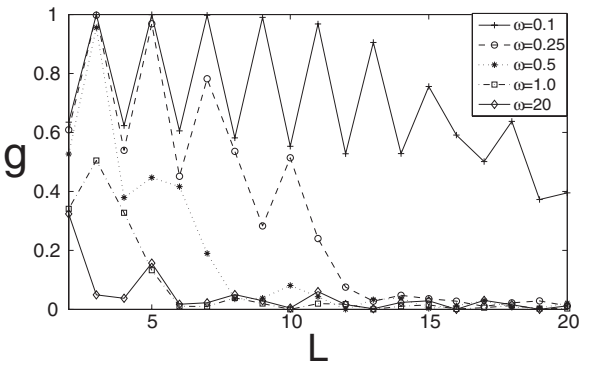

FIG. 6. DC conductance g as a function of the length of the wire for $\Gamma=0.5$, $s=1$, $v/\omega=1$, and for different frequencies.

used, which corresponds to a laser in the near infrared. For the low-frequency regime, a THz laser could be used so that $\hbar\omega=0.1s=0.01$ eV. For the dipole expression to be valid in the time-dependent part of the wire Hamiltonian, the system size should be bigger than the laser wavelength. In the high-frequency case the laser wavelength is of the order of 1 μm. Most molecular wires (except for the longest carbon-nanotubes) would satisfy this condition. For a typical distance of 5 Å between two neighboring sites, a harmonic driving $2v\cos(\Omega t)$ with an amplitude $2v=s$ is equivalent to an electric field strength of 2×10^6 V/cm. A 0.1 W cw-laser focused on an area of $(10\ \mu\text{m})^2$ gives an electric field of 10^4 V/cm, which, after accounting for the amplifying effect of the contacts,[38] would give an amplitude $2v$ in the range of 0.1 eV. These parameters are only a set in the whole range that is experimentally available for exploring the effect of a laser field in the conductance of molecular wires both in the high- and low-frequency regimes.

V. CONCLUSIONS

In this work we have studied the oscillations in the dc conductance of ballistic one-dimensional systems under the effect of an oscillating electric field such as that of a laser beam. The well-known and experimentally observed even-odd oscillations as a function of the system length are substantially modified by the laser field and, in the case of very low frequencies, they can be suppressed due to the localizing effect of a quasi-static electric field. This regime is achieved for driving frequencies smaller than the minimum characteristic energy scale in the Hamiltonian divided by the length of the system. In the high-frequency regime, when the driving frequency is bigger than any energy scale in the Hamiltonian, we observe the effect of dynamic localization, which renormalizes the coupling between sites by a Bessel function $J_0(2v/\hbar\omega)$ and which can produce a zero dc conductance at the zeros of this function. This particular factor only appears in the conductance of systems with an even number of sites, although a length-dependent factor $J_0(2vL/\hbar\omega)$ appears for both even and odd cases introducing additional oscillations as a function of the length. In the general case, using appropriate values of the frequency and amplitude of the laser field we can control the conductance of a quantum wire.

ACKNOWLEDGMENTS

D.F.M. and B.H. acknowledge support from grants from the Hong Kong Research Grants Council and Hong Kong Baptist University. R.A.M.'s contract was financed by the CSIC and the European Commission through the *I3p* Program. This work was supported in part by CAM-CSIC Grant Ref. No. 200650M012.

APPENDIX

As it was explained in the introduction, the even-odd oscillations in half-filled clean quantum wires are a well-known effect that has been measured experimentally. There are different ways of deriving this result and it appears in very different models for the quantum wire. In order to make the paper self-consistent we write in this Appendix a derivation based on Green's functions that will allow us to make direct contact with the analytical results for the Floquet-Green function presented in the main sections. This derivation, to the best of our knowledge, has not been shown before in literature.

Following the discussion about our model in the introduction we can write the clean wire Hamiltonian as

$$H = H_0 + i\Gamma_L|1\rangle\langle 1| + i\Gamma_R|L\rangle\langle L|, \tag{A1}$$

with

$$H_0 = -s\sum_{n=1}^{L-1}(|n\rangle\langle n+1| + |n+1\rangle\langle n|). \tag{A2}$$

The eigenstates of the Hamiltonian H_0 can be constructed using plane waves but including the boundary conditions $\langle 0|\Psi\rangle = 0$ and $\langle L+1|\Psi\rangle = 0$. This can be achieved only if

$$|\Psi_L^n\rangle = N\sum_{l=1}^{L}\sin\frac{n\pi l}{L+1}|l\rangle, \tag{A3}$$

where the index $n = 1, 2, \ldots, L$ and N is a normalization constant, which is found to be $N = \sqrt{2/(L+1)}$. The eigenvalues corresponding to the previous eigenstates can be easily found operating with H (taking into account $\Gamma = 0$) and can be written as a function of quasi-momenta $k_n = n\pi/(L+1)$, $E_n = -2s\cos k_n$.

The components of the Green operator that corresponds to H_0 can be written in terms of the eigenstates and eigenvalues as

$$G_{l,l'}^0(E) = \langle l|\frac{1}{E - H_0}|l'\rangle = \frac{2}{L+1}\sum_n \frac{\sin k_n l \sin k_n l'|l\rangle\langle l'|}{E + 2s\cos k_n}. \tag{A4}$$

In particular, from this expression, the matrix elements $G_{11}^0(E_F)$ and $G_{11}^0(E_F)$ can be shown to be

$$G_{11}^0(0) = \begin{cases} 0 & \text{for } L \text{ even} \\ \infty & \text{for } L \text{ odd} \end{cases},$$

$$G_{1L}^0(0) = \begin{cases} \frac{1}{s}(-1)^{L/2+1} & \text{for } L \text{ even} \\ (-1)^{L-1/2}\infty & \text{for } L \text{ odd}. \end{cases} \tag{A5}$$

In our tight-binding model, and using Landauer's formulation, the conductance can be obtained from the matrix elements of the Green's function,[39] $g = 4\Gamma^2|G_{1L}(E_F)|^2$, valid in one dimension. The result for the Green-function matrix element in the coupled case (H) can be obtained from the result for the uncoupled case (H_0) using Dyson's equation. If $H = H_0 + V$ we can obtain the total Green's function for H from the Green's function of H_0 using $G = G^0 + G^0VG$. For $V = i\Gamma_R|L\rangle\langle L| + i\Gamma_L|1\rangle\langle 1|$, we get $G = G^0 + i\Gamma_R G^0|L\rangle\langle L|G + i\Gamma_L G^0|1\rangle\langle 1|G$, and therefore, the matrix elements that we are interested in are

$$\langle 1|G|L\rangle = G_{1L} = G_{1L}^0 + i\Gamma_L G_{11}^0 G_{1L} + i\Gamma_R G_{1L}^0 G_{LL}, \tag{A6}$$

and

$$\langle L|G|L\rangle = G_{LL} = G_{LL}^0 + i\Gamma_L G_{L1}^0 G_{1L} + i\Gamma_R G_{LL}^0 G_{LL}. \tag{A7}$$

Replacing G_{LL} into the formula for G_{1L} we get, after some algebra,

$$G_{1L} = \frac{G_{1L}^0}{1 - i\Gamma_R G_{LL}^0 - i\Gamma_L G_{11}^0 - \Gamma_L\Gamma_R[G_{11}^0 G_{LL}^0 - (G_{1L}^0)^2]}. \tag{A8}$$

For the Fermi energy in the middle of the band, $K_F = \pi/2$, $E_F = 0$ we can use Eq. (A5) to obtain

$$G_{1L}(0) = \begin{cases} \frac{s(-1)^{L/2+1}}{s^2 + \Gamma_L\Gamma_R} & \text{for L even} \\ \frac{i}{\Gamma_L + \Gamma_R}(-1)^{L-1/2} & \text{for L odd} \end{cases}, \tag{A9}$$

and for $\Gamma_L = \Gamma_R = \Gamma$ we obtain

$$g = \begin{cases} \frac{4\Gamma^2 s^2}{(s^2 + \Gamma^2)^2} & \text{for L even} \\ 1 & \text{for L odd}. \end{cases} \tag{A10}$$

This result is counterintuitive in the limit when $s \to 0$ or $\Gamma \to 0$ since in this case one should expect the conductance of a real system to go to zero both for even and odd number of sites. The problem with this limit lies in the fact that conductance oscillations are obtained under the assumption of coherent transport through the device. This condition would be satisfied in a real system only if the travel time of electrons through the device is much shorter than the typical inelastic scattering time. Clearly, the travel time through the device grows with the inverse of Γ or s (whichever is smaller) and therefore, when taking the limit $s \to 0$ or $\Gamma \to 0$ the effect of inelastic scattering events at some point would become dominant and conductance oscillations would disappear before this limit is reached.

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