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DC voltage profile of a 1D pumped wire with two dynamical and one static impurities

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ABSTRACT

In this work we study the behavior of the voltage profile of a 1D quantum wire with an impurity when transport is induced by two ac voltages that oscillating with a phase lag define a quantum pump. The voltage profile sensed along the wire by the voltage probe, that we assume weakly coupled to the system, exhibits a Friedel's oscillations structure inside the region delimited by the position of the two ac voltages that induce transport. On the other hand, outside this region the oscillations are suppressed. Using perturbation theory in the coupling constant of the voltage probe we derived analytical expressions for the DC current valid for the adiabatic regime. We also compare our analytical results with the exact numerical calculations using Keldysh non-equilibrium Green's functions formalism.

Dynamical transport in mesoscopic structures attracts presently a considerable amount of research. In particular, applying time dependent fields to a mesoscopic conductor opens up new possibilities for electronic transport, specially when the electric fields are time periodic and operate with a phase lag. It is well known that when a phase coherent conductor is subjected to periodically varying voltages a DC current could be pumped even in the absence of a net external bias [1–4].

Several theoretical works have been devoted to study the details of the voltage drop between the contacts in systems where the transport is induced by means of a stationary DC voltage bias [5,6], and as an extension, to study the DC four point resistance (R_{4t}) which could reveal the genuine resistive behavior of the mesoscopic sample [7,8].

However, only recently the analysis of the R_{4t} has been extended to pumping setups. In Ref. [9] we have calculated the voltage profile and the four point resistance of a wire with two barriers at which the ac voltages are applied [9]. We have shown that R_{4t} for the full device, including the barriers coincides with the one obtained in stationary transport, i.e. induced by a DC voltage applied to the reservoirs.

It this communication we analyze an alternative setup where, instead of having two barriers, we have a single impurity within the wire. Our goal is to derive analytical expressions for the DC voltage profile and to determine if the signature of the well known Friedel like oscillations induced by the impurity are still present when transport is induced by quantum pumps. Our analytical calculations could be compared to experimental measurements performed in the adiabatic regime, that is when transport is induced by slowly oscillating fields.

We consider as a model of the quantum pump, a quantum wire coupled to left and right reservoirs at the same fixed chemical potential. Oscillating voltages are applied at two narrow gates with a phase-lag. A fixed impurity, located inside the wire between both quantum pumps serves as an elastic scatterer to the electrons traveling along the sample. The scheme of the setup can be seen in Fig. 1.

The device for a four terminal measurement of the voltage drop consists of two non-invasive voltage probes weakly coupled to the wire. The chemical potential μ_i ($i = P, P'$) of each probe is adjusted to maintain zero net current through the respective contact. As the voltage probes are weakly coupled, the measurement made with one probe is independent of the second one and its location. We start by considering only one voltage probe which is modeled as a third reservoir coupled to the central system at position P. For this system the specific Hamiltonian reads

$$H = H_{leads} + H_P + H_C(t) - w_L(a_L^\dagger c_1 + H.c.) - w_R(a_R^\dagger c_N + H.c.) - w_P(a_P^\dagger c_P + H.c.), \quad (1)$$

with $H_C(t)$ denoting the Hamiltonian for the central piece that we model as a 1D tight-binding chain of length N with two dynamical impurities at sites A and B and one static impurity located at site b:

$$H_C(t) = V\cos(\Omega_0 t + \delta)c_A^\dagger c_A + \sum_{l=1}^{N} \varepsilon_l c_l^\dagger c_l - w_h \sum_{l=1}^{N}(c_l^\dagger c_{l+1} + H.c.) + V\cos(\Omega_0 t)c_B^\dagger c_B, \quad (2)$$

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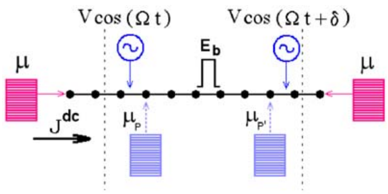

Fig. 1. (Color on-line) Scheme of the setup. The central device is the wire with an impurity at x_b of height E_b, with two out of phase quantum pumps attached at sites x_A and x_B which induce a DC current J^{dc}. The wire is also attached to L and R reservoirs. See text for more details.

with w_h the hopping parameter and the profile $\varepsilon_b = E_b$, $\varepsilon_l = 0$, $l = 1, \ldots, N \neq b$. The time dependent ac potentials act locally at the position of the sites A and B. They oscillate with amplitude V, frequency Ω_0 and phase difference δ. We denote with H_{leads} the Hamiltonians of two semi-infinite tight-binding chains with hopping w_l, which play the role of the L and R reservoirs, which we assume are at the same chemical potential μ. These two leads are connected to the central device at sites $1, N$, respectively. Similarly, H_P is the Hamiltonian of the voltage probe that we also model as a particle reservoir with chemical potential μ_P that is fixed to satisfy the condition of net zero DC current through the probe P [10]. The contacts between the central system and the L and R leads and the probe P are described by the last three terms of Eq. (1), where the fermionic operators a_α ($\alpha = L, R, P$) denote degrees of freedom for the L, R and P reservoirs, respectively.

We employ the formalism of Keldysh non-equilibrium Green's functions technique, which is a convenient tool in transport theory on multiterminal structures driven by time-periodic fields [4]. Following Ref. [4] we employ the Floquet representation $G^R_{l,l'}(t,\omega) = \sum_{k=-\infty}^{\infty} \mathscr{G}(k,\omega) e^{-ik\Omega_0 t}$ where $G^R_{l,l'}(t,\omega)$ is the Fourier transform with respect to $t - t'$ of the retarded Green's function. The DC component of the charge current flowing through a lead from the central system towards the probe P, can be written (in units of e/h) as [4]

$$J^{dc}_P = \sum_{\alpha=L,P,R} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \{ \Gamma_\alpha(\omega) \Gamma_P(\omega + k\Omega_0) \times |\mathscr{G}_{l_P, l_\alpha}(k,\omega)|^2 [f_\alpha(\omega) - f_P(\omega + k\Omega_0)] \}, \quad (3)$$

where l_α are the sites of the central system at which the reservoirs $\alpha = L, R, P$ are attached, while $\Gamma_\alpha(\omega) = |w_\alpha|^2 \rho_\alpha(\omega)$ is the spectral function associated to the self-energies due to the coupling to these reservoirs. $\rho_\alpha(\omega)$ is the corresponding density of states and $f_\alpha(\omega) = 1/(e^{\beta_\alpha(\omega - \mu_\alpha)} + 1)$ the Fermi function of the reservoir α, which we assume to be at the temperature $1/\beta_\alpha = 0$.

The voltage profile sensed by the probe can be exactly evaluated under general conditions from the solution μ_P that satisfies $J^{dc}_P = 0$ in the above expression. To derive analytical expressions for the voltage profile we analyze the case of low driving frequency Ω_0 and small pumping amplitude V [2].

As we already mentioned, we are interested in the behavior of the voltage profile sensed by "non-invasive probes". This corresponds to probes weakly coupled to the central system, in such a way that they do not introduce neither inelastic nor elastic scattering processes for the electronic propagation between L and R reservoirs. Below we derive an analytical expression, valid under these conditions, for the voltage profile μ_P.

In order to obtain the expressions for the Green's functions we solved perturbatively, up to first order in the pumping amplitude V, the Dyson's equation using the Floquet representation [4]:

$$\mathscr{G}_{l,l'}(0,\omega) \sim G^0_{l,l'}(\omega),$$

$$\mathscr{G}_{l,l'}(\pm 1,\omega) \sim \frac{V}{2} [G^0_{l,A}(\omega \mp \Omega_0) G^0_{A,l'}(\omega) + e^{\pm i\delta} G^0_{l,B}(\omega \mp \Omega_0) G^0_{B,l'}(\omega)]. \quad (4)$$

For weak coupling to the probes, Eq. (3) is evaluated with Green's functions up to the first order in w_P. After imposing the condition of zero net DC current and using the fact that only Floquet components with $k = 0, \pm 1$ enter in Eq. (4), the voltage sensed by the probe P casts

$$\mu_P = \mu + \Omega \left(\frac{V w_h \sin\theta}{2} \right)^2 [|\mathscr{G}_{P,1}(1,\omega)|^2 + |\mathscr{G}_{P,N}(1,\omega)|^2 - |\mathscr{G}_{P,1}(-1,\omega)|^2 - |\mathscr{G}_{P,N}(-1,\omega)|^2]. \quad (5)$$

At the lowest order of perturbation in w_P, the functions $G^0_{l,l'}(\omega)$ entering the above expressions are the equilibrium retarded Green's functions of the central system attached only to the L and R reservoirs. For perfect matching to the reservoirs ($w_L = w_R = w_l = w_h$) and for an static impurity with low amplitude $E_b \leqslant w_h$, these functions can be written in the following simple form: $G^0_{l,l'}(\omega) = g_{l,l'}(\theta) + E_b g_{l,b}(\theta) g_{b,l'}(\theta)$, with $g_{l,l'}(\theta) = i\, e^{-i|l-l'|\theta}/(2w_h \sin\theta)$, being $\omega = 2w_h \cos\theta$ [12]. Using these Green's functions to evaluate Eq. (4), substituting the result in Eq. (3) and considering the adiabatic ($\propto \Omega_0$) contribution in the resulting J^{dc}_P we get when the probe is located outside the pumping centers:

$$\mu^o_P = \mu \pm \Omega_0 V^2 \sin\delta [(2w_h \sin k_F) \hat{\alpha}(2x_A, k_F) - E_b \alpha(x_b, k_F)], \quad x_P > x_B, \; x_P < x_A, \quad (6)$$

and

$$\mu^i_P = \mu - \Omega_0 V^2 \sin\delta [\beta(x_P, k_F) - E_b(\alpha(x_P, k_F) \pm \hat{\beta}(x_b, k_F) \mp \hat{\beta}(x_P, k_F))], \quad x_A < x_P < x_B, \; x_P > x_b, \; x_P < x_b \quad (7)$$

for the case in which the probe is located between the two pumping centers. We denote by x_j ($j = A, B, P, b$) the position of the pumps, the probe and the static impurity, respectively, in units of the lattice parameter of the tight-binding model. The upper and lower signs of Eq. (6) correspond, respectively, to the voltage probe located at the left ($x_P < x_A$) and at the right ($x_P > x_B$) side of the pumping region. In Eq. (7) the upper and lower signs correspond to the voltage probe located between the pumps at the left ($x_P < x_b$) and at the right ($x_P > x_b$) side of the static impurity, respectively.

We have defined the Fermi vector (in units of the lattice parameter) as $k_F \equiv \theta(\mu)$ as well as the following functions:

$$\alpha(x, k_F) = \frac{\sin[k_F(x_A - x_B)] \sin[k_F(2x - x_A - x_B)]}{(2w_h \sin k_F)^3},$$
$$\hat{\alpha}(x, k_F) = \frac{\sin[k_F(x_A - x_B)] \cos[k_F(2x - x_A - x_B)]}{(2w_h \sin k_F)^3},$$
$$\beta(x, k_F) = \frac{\cos[k_F(x_A - x_B)] \sin[k_F(2x - x_A - x_B)]}{(2w_h \sin k_F)^3},$$
$$\hat{\beta}(x, k_F) = \frac{\cos[k_F(x_A - x_B)] \cos[k_F(2x - x_A - x_B)]}{(2w_h \sin k_F)^3}. \quad (8)$$

Fig. 2 shows the benchmark of the analytical result, Eqs. (6) and (7), against the exact voltage profile obtained numerically from Eq. (11) in the regime of weak V, Ω_0 and w_P, and a moderate E_b. A good agreement of the qualitative behavior is observed. In particular, the exact profile μ_P exhibits Friedel's oscillations with period $2k_F$ as a function of the probe position x_P as predicted by Eq. (7) and only a slight disagreement is found in the amplitude of the envelope function.

Within the lowest order of perturbation in the coupling constant w_P, the effect of an additional second voltage probe P' can be considered completely uncorrelated from the first one, since the associated interference effects involve second order

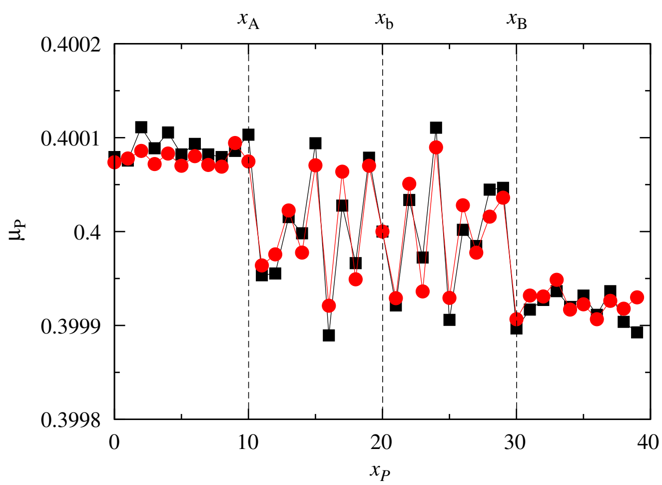

Fig. 2. Local voltage μ_P sensed by the voltage probe P as a function of the probe position x_P along the 1D wire of $N = 40$ sites with an impurity of height $E_b = 0.2$ located at $x_b = 20$. The positions of the two quantum pumps at $x_A = 10$ and $x_B = 30$ are indicated by the vertical dashed lines. The pumping parameters are $V = 0.01$, $\Omega_0 = 0.01$ and $\delta = \pi/2$. Red squares correspond to Eqs. (6)–(7) the analytical solution for the adiabatic pumping regime and a weakly connected probe. Black circles correspond to the exact numerical solution obtained equating Eq. (3) to zero with $w_P = 0.01$. The chemical potential is $\mu = 0.4$, which corresponds to $k_F = 1.36$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

processes in w_P. At this level of approximation let us call $\mu_{P'}$ the local voltage sensed by the additional probe at P' and $\Delta\mu_{PP'} \equiv \mu_{P'} - \mu_P$ the corresponding voltage drop. In a setup in which the probe P is located at the left side of x_A and the probe P' at the right side of x_B, the voltage drop between both probes is, from Eq. (7),

$$\Delta^o \mu_{PP'} = 2\Omega_0 V^2 \sin\delta\{(2w_h \sin k_F)\hat{\alpha}(2x_A, k_F) + E_b[\alpha(2x_B, k_F) + \hat{\beta}(x_b, k_F)]\}. \tag{9}$$

Another possible measurement corresponds to locate the voltage probes P and P' inside the region delimited by the quantum pumps at both sides of the static impurity. In this case, the voltage drop between the two probes explicitly depends on the probe positions x_P and $x_{P'}$ as follows:

$$\Delta^i \mu_{PP'} = 2\Omega_0 V^2 \sin\delta\{(2w_h \sin k_F)\hat{\beta}(\bar{x}, k_F) \times \sin(k_F \Delta x) + E_b[\hat{\beta}(\bar{x}, k_F)\sin(k_F \Delta x) + \beta(\bar{x}, k_F)\sin(k_F \Delta x) + \hat{\alpha}(\bar{x}, k_F)\cos(k_F \Delta x)]\}, \tag{10}$$

with

$$\bar{x} = \frac{x_P + x_{P'}}{2}, \quad \Delta x = x_P - x_{P'},$$

where, as before, we have employed the superscripts $o, (i)$ to distinguish configurations with the probes outside (inside) the pumps (located at x_A and x_B).

Interestingly, Eq. (7) shows the characteristic pattern of the Friedel oscillations with a period $2k_F$, and remarkably these oscillations are only present at positions lying between the two quantum pumps. In fact the oscillatory terms of expressions of Eq. (6)–(7) depend on the position of the static scatterer, x_b, and on the pumping positions x_A and x_B. Notice, however, that these Friedel's oscillations can be identified as interference processes involving the static *as well as the two dynamical* impurities. This is in contrast with the behavior found for the Friedel's oscillations induced by a single static impurity under stationary driving [11], which only depend on the position of the impurity. On the other hand, the voltage drop measured when both probes are located outside the pumping region does not depend on the specific position, and its sign determines the direction of the DC current. Under the conditions assumed in the derivation of Eq. (7), i.e. low V, Ω_0, w_P and E_b, the DC current flowing through wire reads

$$J^{dc} \cong \frac{4\Gamma_L^0 \Gamma_R^0 \Omega_0 V^2 \sin\delta}{(2w_h \sin k_F)^2}\{w_h(\sin k_F)\alpha(2x_B, k_F) + E_b[\alpha(x_A, k_F) - \beta(2x_A, k_F) - \hat{\beta}(2x_b, k_F)]\}, \tag{11}$$

with $\Gamma_\alpha^0 \equiv \Gamma_\alpha^0(\mu)$, $\alpha = L, R$.

The four terminal resistance can be evaluated straightforwardly by evaluating the quotient between Eqs. (10) and (11). Unlike the case considered in our previous work [9] this estimate of R_{4t} does not coincide with the corresponding one to a single impurity placed between two stationary reservoirs with an equivalent voltage difference. The reason is that the interference effects introduced in the pumping setup by the two additional dynamical impurities cannot be captured in the stationary setup.

To conclude we have derived analytical expressions for the dc voltage profile and the DC current of a quantum pump with an static impurity valid in the adiabatic regime. At this level of approximation we found that the Friedel's oscillations sensed by the voltage probes appear only inside the region delimited by the quantum pumps, while the voltage measured outside this region remains constant and unambiguously determines the direction of the dc current. We have found a good agreement between our analytical expressions derived for weak driving and the results of the exact numerical calculations. However, the result for R_{4pt} is different from the one corresponding to the stationary counterpart.

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