

Adiabatic quantum pump in the presence of external ac voltages

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(Received 28 September 2003; revised manuscript received 18 November 2003; published 26 May 2004)

We investigate a quantum pump which in addition to its dynamic pump parameters is subject to oscillating external potentials applied to the contacts of the sample. Of interest is the rectification of the ac currents flowing through the mesoscopic scatterer and their interplay with the quantum pump effect. We calculate the adiabatic dc current arising under the simultaneous action of both the quantum pump effect and classical rectification. In addition to two known terms we find a third contribution which arises from the interference of the ac currents generated by the external potentials and the ac currents generated by the pump. The interference contribution renormalizes both the quantum pump effect and the ac rectification effect. Analysis of this interference effect requires a calculation of the Floquet scattering matrix beyond the adiabatic approximation based on the frozen scattering matrix alone. The results permit us to find the instantaneous current. In addition to the current generated by the oscillating potentials, and the ac current due to the variation of the charge of the frozen scatterer, there is a third contribution which represents the ac currents generated by an oscillating scatterer. We argue that the resulting pump effect can be viewed as a quantum rectification of the instantaneous ac currents generated by the oscillating scatterer. These instantaneous currents are an intrinsic property of a nonstationary scattering process.

DOI: 10.1103/PhysRevB.69.205316

PACS number(s): 72.10.-d, 73.23.-b, 73.40.Ei

I. INTRODUCTION

Dynamical transport in mesoscopic structures attracts presently considerable attention.¹⁻¹² In particular, the possibility to vary several parameters at the same frequency but different phases⁷ of a mesoscopic system opens up new prospects for the investigation of quantum transport. Applying two slowly oscillating potentials at frequency ω with fixed phase lag $\Delta\varphi$ to a mesoscopic conductor connected to reservoirs having equal electrochemical potentials one can generate an adiabatic dc current

$$I_{dc} \sim \omega \sin(\Delta\varphi). \quad (1)$$

Such a current was measured experimentally.⁷ However, the precise origin of the measured current is still unclear. At least two mechanisms considered in the literature can contribute to the experimentally measured current (see Fig. 1). First, there exists a *quantum pump effect*^{7,13-46} which is due to quantum-mechanical interference and dynamical breaking of time-reversal invariance. Second, there also exists a *rectification of ac currents* by the oscillating scatterer^{12,47,48} if it is part of an external circuit with nonzero impedance. Closely related to this second effect is a pump in the presence of inelastic scattering: in addition to the externally driven pump parameters, inelastic scattering leads to an effective oscillating (electro)chemical potential of the pump which acts like an additional pump parameter.⁴⁹

We stress that from the physical point of view the oscillating electrochemical potentials (external voltages) differ essentially from the oscillating pump parameters (internal voltages). If the latter affect only the outgoing carriers the former affect the incoming carriers. The distinction between external voltages and internal potentials is also central in theories of

ac conductance.¹ Here, this distinction helps us to perform detailed partitioning of the current generated by the pump [see Eqs. (33) and (38)].

The aim of the present paper is to investigate both above-mentioned mechanisms on the same footing. To this end we consider a phase-coherent oscillating scatterer coupled to reservoirs with oscillating potentials (Fig. 1). We will show that in general the above-mentioned mechanisms do not simply add but interfere between themselves. This leads to a renormalization of both the quantum pump effect as well as the rectification effect in the total dc current. To find this additional interference contribution we go beyond the frozen scattering matrix approximation and take into account the

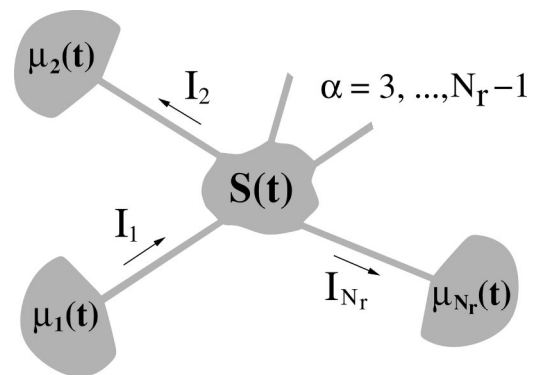


FIG. 1. A mesoscopic pump with scattering matrix $S(t)$ oscillating with frequency ω is coupled to N_r reservoirs with electrochemical potentials $\mu_\alpha(t)$ oscillating with the same frequency ω . A quantum pump effect and a classical rectification effect together result in dc currents I_α flowing through the scatterer. The full current is time dependent and is needed to characterize pumps in a nonzero impedance external circuit.

first order in pump frequency corrections to the scattering matrix. The necessity to include such corrections in a general case emphasizes that the quantum adiabatic pump effect is an essentially “nonadiabatic” phenomenon.³⁰

Theoretically, quantum pumps have been investigated mostly under the (implicit) condition that the external circuit exhibits zero impedance. The work of Brouwer,⁴⁷ Polianski and Brouwer,⁴⁸ the work on inelastic scattering⁴⁹ mentioned already, and the recent work of Martinez-Mares, Lewenkopf, and Mucciolo⁵⁰ represent the few exceptions. In reality the zero-impedance condition seems never exactly fulfilled. Coupling an oscillating gate voltage to a scatterer leads, due to the long-range nature of the Coulomb interaction, effectively to oscillating voltages at all terminals.¹² In addition, in experiments, the pump is investigated with an impedance in series with the oscillating scatterer. Furthermore, a voltage probe, to maintain zero current in the presence of pumping, in effect generates an oscillating potential which acts back on the pump.⁴⁹ Therefore, for theory to make contact with experiment, it is necessary to consider the effect of oscillating voltages at the contacts of the conductor.

The paper is organized as follows. In Sec. II we develop the Floquet scattering matrix approach for ac quantum transport through the nonstationary (oscillating) scatterer in the presence of oscillating reservoir potentials. A full theory requires even to first order in frequency an investigation of nonadiabatic corrections to the adiabatic (frozen) scattering matrix. These corrections are discussed in Sec. III. The current to linear order in the reservoir potentials is calculated in Sec. IV. We illustrate the results for a simple one-channel scatterer with two contacts. In Sec. V we present a general expression for the current valid for finite potentials. Section VI gives the expression for the instantaneous current.

II. GENERAL APPROACH

For simplicity we consider here the mesoscopic sample, the pump, connected to N_r reservoirs via single channel leads (Fig. 1). We are interested in the dc and ac currents flowing in the system if this system is subject to a cyclic evolution with period \mathcal{T} . The general situation we want to consider admits the scatterer and the reservoir properties to be oscillating with frequency $\omega = 2\pi/\mathcal{T}$.

We use the scattering matrix approach to ac transport in phase-coherent mesoscopic systems.¹ According to this approach the currents flowing in the system are determined by the scattering of electrons coming from the reservoirs by the mesoscopic sample.^{51,52} In the present paper we deal with noninteracting electrons. A full theory has eventually to treat the internal potential of the pump in a self-consistent manner.

The scattering properties of a mesoscopic sample oscillating with frequency ω can be described via the Floquet scattering matrix \hat{S}'_F (see, e.g., Ref. 30).

The matrix element $S'_{F,\alpha\beta}(E_n, E)$ is a quantum-mechanical amplitude for an electron with energy E entering the scatterer through lead β to leave the scatterer through lead α having energy $E_n = E + n\hbar\omega$. We use Greek letters α ,

β to number the leads connecting the scatterer to the reservoirs: $\alpha, \beta = 1, \dots, N_r$.

Denoting by \hat{a}' an annihilation operator for incoming particles we can write down the expression for the annihilation operators \hat{b}' for outgoing particles,^{30,26,52}

$$\hat{b}'_{\alpha}(E) = \sum_{\beta} \sum_{E_n > 0} S'_{F,\alpha\beta}(E, E_n) \hat{a}'_{\beta}(E_n). \quad (2)$$

By definition the reservoirs are not affected by the coupling to the scatterer and thus they are in an equilibrium (but not necessary stationary) state. Therefore the properties of incoming particles are independent of the scatterer and are determined by the reservoirs. To be definite we suppose that the cyclic evolution of any reservoir α is due to solely an oscillating electrochemical potential $\mu_{\alpha}(t)$:

$$\begin{aligned} \mu_{\alpha}(t) &= \mu_{0,\alpha} + eV_{\alpha}(t), \\ V_{\alpha}(t) &= V_{\alpha} \cos(\omega t + \varphi_{\alpha}), \end{aligned} \quad (3)$$

$$eV_{\alpha} \ll \mu_{0,\alpha}.$$

We emphasize that we must keep track of the phase shifts φ_{α} since there are a number of oscillating potentials and we cannot eliminate all the phases φ_{α} simultaneously by merely shifting the time origin.

It is well known (see, e.g., Ref. 53) that the wave functions for free electrons in the reservoir (say, α) with an oscillating uniform potential $V_{\alpha}(t)$ are of the Floquet function type:

$$\psi_{\alpha}(E, t, \mathbf{r}) = e^{i\mathbf{k}\mathbf{r} - iEt/\hbar} \sum_{n=-\infty}^{\infty} J_n\left(\frac{eV_{\alpha}}{\hbar\omega}\right) e^{-in(\omega t + \varphi_{\alpha})}. \quad (4)$$

Here $J_n(x)$ is the Bessel function of the first kind of the n th order; $E = \hbar^2 k^2 / (2m_e)$ (m_e is an electron mass). The corresponding distribution function $f_{0,\alpha} = \langle \hat{a}'_{\alpha}(E) \hat{a}_{\alpha}(E) \rangle$ (here $\langle \dots \rangle$ means quantum-statistical averaging) is independent of the oscillating potential V_{α} and is the Fermi distribution function

$$f_{0,\alpha}(E) = \frac{1}{1 + \exp\left(\frac{E - \mu_{0,\alpha}}{k_B T_{\alpha}}\right)}. \quad (5)$$

Here T_{α} is the temperature of the reservoir α ; k_B is the Boltzman constant.

In general, to find the Floquet scattering matrix \hat{S}'_F , we have to investigate the transmission and reflection amplitudes of electrons with a wave function $\psi(E, t, \mathbf{r})$ given by Eq. (4) incident on the oscillating scatterer. However, if the frequency ω is small compared with the energy of electrons participating in the transport (i.e., with the Fermi energy μ)

$$\hbar\omega \ll \mu, \quad (6)$$

we can reduce the problem to scattering of ordinary plane waves. To this end we use the following trick.⁵³ We imagine

that in the leads connecting scatterer to the reservoirs the oscillating potentials tend to zero: $V_\alpha=0$. Then in the leads the electron wave functions are simply plane waves,

$$\psi_{0,\alpha}(E, r) = e^{i\mathbf{k}r - iEt/\hbar}. \quad (7)$$

In this region we introduce annihilation operators \hat{a} , \hat{b} for incoming and outgoing particles, respectively. In close analogy with Eq. (2) they are related but through the Floquet scattering matrix $S_{F,\alpha\beta}(E_n, E)$ describing scattering of incident and outgoing plane waves:

$$\hat{b}_\alpha(E) = \sum_\beta \sum_n S_{F,\alpha\beta}(E, E_n) \hat{a}_\beta(E_n). \quad (8)$$

Comparing the wave functions, Eqs. (4) and (7), we see that the annihilation operators \hat{a} for particles in the leads can be expressed in terms of the annihilation operators \hat{a}' for particles in the reservoirs as follows:⁵³

$$\hat{a}_\alpha(E) = \sum_{n=-\infty}^{\infty} J_n \left(\frac{eV_\alpha}{\hbar\omega} \right) e^{-in\varphi_\alpha} \hat{a}'_\alpha(E - n\hbar\omega). \quad (9)$$

The above representation is valid for small frequencies, Eq. (6). Thus we can put $k(E_n) \approx k(E)$ ignoring the terms of order $\hbar\omega/\mu$ and smaller. In other words we ignore the reflection at the interface between the region with oscillating potential and the region without one.

Using Eqs. (8) and (9) we calculate the distribution functions $f_\alpha^{(out)}(E) = \langle \hat{b}_\alpha^\dagger(E) \hat{b}_\alpha(E) \rangle$ for outgoing and $f_\alpha^{(in)}(E) = \langle \hat{a}_\alpha^\dagger(E) \hat{a}_\alpha(E) \rangle$ for incoming electrons in the leads as follows:

$$f_\alpha^{(in)}(E) = \sum_{n=-\infty}^{\infty} J_n^2 \left(\frac{eV_\alpha}{\hbar\omega} \right) f_{0,\alpha}(E - n\hbar\omega), \quad (10a)$$

$$\begin{aligned} f_\alpha^{(out)}(E) &= \sum_\beta \sum_{n,m,q=-\infty}^{\infty} S_{F,\alpha\beta}^*(E, E_q) S_{F,\alpha\beta}(E, E_m) \\ &\times J_{n+q} \left(\frac{eV_\beta}{\hbar\omega} \right) J_{n+m} \left(\frac{eV_\beta}{\hbar\omega} \right) e^{i(q-m)\varphi_\beta} \\ &\times f_{0,\beta}(E - n\hbar\omega). \end{aligned} \quad (10b)$$

Now the dc current I_α of spinless electrons, the quantity of interest here, flowing from the scatterer through the lead α can be expressed in terms of these distributions,²⁶

$$I_\alpha = \frac{e}{h} \int_0^\infty dE \{ f_\alpha^{(out)}(E) - f_\alpha^{(in)}(E) \}. \quad (11)$$

Substituting Eq. (10) into Eq. (11) we find

$$\begin{aligned} I_\alpha &= \frac{e}{h} \int_0^\infty dE \sum_\beta \sum_{n=-\infty}^{\infty} f_{0,\beta}(E - n\hbar\omega) \\ &\times \left\{ \sum_{m,q=-\infty}^{\infty} S_{F,\alpha\beta}^*(E, E_q) S_{F,\alpha\beta}(E, E_m) \right. \\ &\times J_{n+q} \left(\frac{eV_\beta}{\hbar\omega} \right) J_{n+m} \left(\frac{eV_\beta}{\hbar\omega} \right) e^{i(q-m)\varphi_\beta} - \delta_{\alpha\beta} J_n^2 \left(\frac{eV_\alpha}{\hbar\omega} \right) \left. \right\}. \end{aligned} \quad (12)$$

Equation (12) is the basic result which allows us to analyze the dc currents flowing in the system under consideration. So far we put no restrictions on the reservoirs. Different temperatures of reservoirs as well as different (stationary) electrochemical potentials can by themselves give rise to dc currents. We will not consider the most general situation here. Pumping in the presence of stationary chemical potential differences is investigated by Entin-Wohlman *et al.*^{25,46} Here we focus on dynamically oscillating potentials.

In what follows we assume the reservoirs to have equal temperatures and equal dc components of electrochemical potentials but the oscillating reservoir potentials V_α can be different:

$$T_\alpha = T_0, \quad \mu_{0,\alpha} = \mu_0, \quad \alpha = 1, \dots, N_r. \quad (13)$$

In this case the distribution functions entering Eq. (12) are independent of the lead index: $f_{0,\alpha(\beta)}(X) = f_0(X)$, where f_0 is the Fermi distribution function with temperature T_0 and chemical potential μ_0 .

To calculate the Floquet scattering matrix $\hat{S}_F(E, E_n)$ one needs to solve the time-dependent scattering problem. Generally this can be done only numerically (see, e.g., Ref. 30).

Here we are interested in the limit of low frequencies. In this limit we can use the adiabatic approximation as a starting point and can express the Floquet scattering matrix in terms of a stationary scattering matrix with time-dependent parameters (the *frozen* scattering matrix): $\hat{S}_0(E, t) \equiv \hat{S}_0(E, \{P(t)\})$. Here $\{P\}$ is a set of parameters $P_i(t) = P_{i,0} + P_{i,1} \cos(\omega t + \phi_i)$, $i=1, 2, \dots, N_p$ oscillating with frequency ω . The scattering matrix $\hat{S}_0(E, \{P\})$ describes reflection and transmission of particles with energy E at given frozen parameters P_i . This description is valid if the energy scale $\hbar\omega$ dictated by the modulation frequency is small compared with the energy scale δE over which the scattering matrix $\hat{S}(E)$ changes significantly.³⁰

III. ADIABATIC APPROXIMATION

To zeroth order in frequency the elements of the Floquet scattering matrix can be approximated by the Fourier coefficients $\hat{S}_{0,n}$ of the stationary scattering matrix \hat{S}_0 ,

$$\hat{S}_{0,n}(E) = \frac{\omega}{2\pi} \int_0^T dt e^{in\omega t} \hat{S}_0(E, t), \quad (14a)$$

$$\hat{S}_0(E, t) = \sum_{n=-\infty}^{\infty} e^{-in\omega t} \hat{S}_{0,n}(E), \quad (14b)$$

as follows:³⁰

$$\hat{S}_F(E_n, E) \approx \hat{S}_F(E, E_{-n}) \approx \hat{S}_{0,n}(E). \quad (15)$$

However, in general this approximation is not sufficient to calculate the current to order ω . In particular, if the oscillating potentials $V_\alpha \neq 0$ are applied to the reservoirs then to calculate the dc current to first order in frequency ω one needs to know the Floquet scattering matrix with the same accuracy.

Note that fortunately in the case of stationary reservoirs ($V_\alpha = 0$) there exists a representation [see Eq. (8) in Ref. 30] which allows to calculate the dc current (with accuracy of order ω) using only the zero-order approximation, Eq. (15). In contrast, another representation [see Eq. (9) in Ref. 30] for the same dc current requires the knowledge of the Floquet scattering matrix with higher accuracy (i.e., to the first order in frequency).

Note that the nonadiabatic corrections to the scattering states and the corresponding corrections to the pumped current were considered in Refs. 25 and 46 in the limit of a small modulating potential. Our approach is valid for an arbitrary oscillating potential since we take into account the effect of all the harmonics of the pump frequency ω .

To calculate the Floquet scattering matrix with an accuracy of order ω we generalize the approach used in Ref. 1 and start from the unitarity conditions for the Floquet scattering matrix:³⁰

$$\sum_{\alpha} \sum_{n=-\infty}^{\infty} S_{F,\alpha\beta}^*(E_n, E) S_{F,\alpha\gamma}(E_n, E_m) = \delta_{m0} \delta_{\beta\gamma}, \quad (16a)$$

$$\sum_{\beta} \sum_{n=-\infty}^{\infty} S_{F,\alpha\beta}^*(E, E_n) S_{F,\gamma\beta}(E_m, E_n) = \delta_{m0} \delta_{\alpha\gamma}. \quad (16b)$$

Taking into account that Eq. (15) is a zeroth-order approximation we will seek the first-order approximation in the following form:

$$\hat{S}_F(E_n, E) = \hat{S}_{0,n} \left(\frac{E_n + E}{2} \right) + \hbar \omega \hat{A}_n(E) + O(\omega^2), \quad (17a)$$

$$\hat{S}_F(E, E_{-n}) = \hat{S}_{0,n} \left(\frac{E + E_{-n}}{2} \right) + \hbar \omega \hat{A}_n(E) + O(\omega^2). \quad (17b)$$

Here $\hat{A}_n(E)$ is a matrix of the Fourier coefficients for some matrix $\hat{A}(E, t) \equiv \hat{A}(E, \{P(t)\})$ which is treated as independent of energy on the scale of the order of $n\hbar\omega$; $O(\omega^2)$ denotes the rest which is at least of second order in frequency ω and which we neglect. Note that the first terms in Eqs. (17) should be expanded to the first order in ω :

$$\hat{S}_{0,n} \left(\frac{E + E_{\pm n}}{2} \right) \approx \hat{S}_{0,n}(E) \pm \hbar \omega \frac{n}{2} \frac{\partial \hat{S}_{0,n}(E)}{\partial E},$$

and other terms (of higher order in ω) should be ignored.

Based on Eq. (21) we will show that Eq. (17) is, in fact, an expansion in powers of $\hbar\omega/\delta E$. Substituting Eqs. (17) into Eqs. (16) and keeping the terms of order ω^0 and ω^1 we get the required relations which can be used to calculate the current, Eq. (12).

In particular the diagonal part ($m=0, \beta=\gamma$) of Eqs. (16) gives

$$\begin{aligned} & \sum_{\alpha(\beta)} \sum_{n=-\infty}^{\infty} S_{0,\alpha\beta,n}^*(E) A_{\alpha\beta,n}(E) + \text{c.c.} \\ & = \mp \frac{1}{2} \frac{\partial}{\partial E} \sum_{\alpha(\beta)} \sum_{n=-\infty}^{\infty} n |S_{0,\alpha\beta,n}(E)|^2. \end{aligned} \quad (18)$$

Here c.c. denotes complex-conjugate terms. The sign $-$ ($+$) corresponds to the summation over $\alpha(\beta)$.

In what follows, we mainly concentrate on the case without magnetic fields and suppose that the stationary scattering matrix is symmetric in lead indices:

$$S_{0,\alpha\beta} = S_{0,\beta\alpha}. \quad (19)$$

It follows from Eq. (18) that in this case the matrix \hat{A} is antisymmetric:

$$A_{\alpha\beta} = -A_{\beta\alpha}. \quad (20)$$

Since $A_{\alpha\alpha} = 0$, we can immediately conclude that the reflection ($\alpha=\beta$) coefficients are with accuracy of order ω defined by the first terms on the right-hand side (RHS) of Eqs. (17). This fact justifies our representation for the elements of the Floquet scattering matrix in Eqs. (17).

We next need to determine the off-diagonal elements of \hat{A} . The detailed calculation is given in the Appendix. The central result is the relation (valid to first order in ω)

$$\hbar \omega [\hat{S}_0^\dagger(E, t) \hat{A}(E, t) + \hat{A}^\dagger(E, t) \hat{S}_0(E, t)] = \frac{1}{2} \mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}, \quad (21a)$$

$$\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\} = i\hbar \left(\frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E} - \frac{\partial \hat{S}_0^\dagger}{\partial E} \frac{\partial \hat{S}_0}{\partial t} \right). \quad (21b)$$

Here i is the imaginary unit. Since the scattering matrix is unitary $\hat{S}_0^\dagger \hat{S}_0 = \hat{I}$ (where \hat{I} is a unit matrix) the matrix $\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}$ is traceless: $\sum_{\alpha=1}^{N_r} \mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}_{\alpha\alpha} = 0$ (see the Appendix for the detailed proof).

Note Avron *et al.*⁴⁰ consider a closely related matrix $\hat{\Omega} = \mathcal{P}\{\hat{S}_0; \hat{S}_0^\dagger\}$. This matrix is the commutator $\hat{\Omega} = i/\hbar [\hat{\mathcal{T}}, \hat{\mathcal{E}}]$ of the Wigner time-delay matrix:^{54,55} $\hat{\mathcal{T}} = -i\hbar(\partial \hat{S}_0 / \partial E) \hat{S}_0^\dagger$, and the matrix of the energy shift:^{22,40} $\hat{\mathcal{E}} = i\hbar(\partial \hat{S}_0 / \partial t) \hat{S}_0^\dagger$. Note, however, that on the RHS of Eq. (21a) the commutator appears with a different sequence of \hat{S}_0^\dagger and \hat{S}_0 as compared to $\hat{\Omega}$. For this reason (and other reasons to become clear later

on, we have introduced a separate notation, the Poisson bracket \mathcal{P} . As we will show [see Eq. (34)] the diagonal elements $(e/h)\mathcal{P}\{\hat{S}_0; \hat{S}_0^\dagger\}_{\alpha\alpha}$ are just spectral current densities (current per energy).

If the matrix \hat{S}_0 is a symmetric 2×2 matrix ($N_r=2$) then from Eq. (21a) we can find an expression for the product of the frozen scattering matrix with elements of \hat{A} ,

$$4\hbar\omega \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] = \frac{1}{2} [\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}_{\beta\beta} - \mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}_{\alpha\alpha}]. \quad (22a)$$

Otherwise we can only conclude that

$$4\hbar\omega \sum_{\alpha=1}^{N_r} \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] = \mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}_{\beta\beta}, \quad (22b)$$

$$4\hbar\omega \sum_{\beta=1}^{N_r} \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] = \mathcal{P}\{\hat{S}_0; \hat{S}_0^\dagger\}_{\alpha\alpha}. \quad (22c)$$

Here $\text{Re}[X]$ is a real part of X . To get Eq. (22c) we multiplied Eq. (21a) from the left by \hat{S}_0 , and from the right by \hat{S}_0^\dagger , and used the unitarity condition $\hat{S}_0 \hat{S}_0^\dagger = \hat{S}_0^\dagger \hat{S}_0 = \hat{I}$.

Below we use Eqs. (17) and (22) to evaluate the current Eq. (12) with an accuracy of order ω .

IV. LINEAR-RESPONSE ADIABATIC CURRENT

Now we use the adiabatic approximation introduced in the preceding section and calculate the zero-frequency, dc current [Eq. (12)] to linear order in the oscillating potentials $V_\alpha \rightarrow 0$ of the reservoirs at finite temperature T_0 . We assume that the following conditions hold:

$$\hbar\omega \ll k_B T_0, \quad (23a)$$

$$eV_\alpha \ll k_B T_0. \quad (23b)$$

The first inequality ($\hbar\omega \ll k_B T_0$) is relevant for experiments on adiabatic ($\omega \rightarrow 0$) quantum transport. The second inequality defines nothing but the linear-response regime.

In Eq. (12) the sum over n contains approximately $n_{\max} \sim (eV/\hbar\omega)$ terms. Therefore, $\hbar\omega n \ll eV$ and because of Eq. (23b) we have $\hbar\omega n \ll k_B T$. Hence we can expand the Fermi function entering Eq. (12). Taking into account Eq. (13) this expansion (up to second order in ω) is $f_{0,\beta}(E - n\hbar\omega) \approx f_0(E) - n\hbar\omega [\partial f_0(E)/\partial E] + \frac{1}{2} n^2 \hbar^2 \omega^2 [\partial^2 f_0(E)/\partial E^2]$. Substituting this distribution into Eq. (12), take the sum over n . We use the summation formulas for the Bessel functions:⁵⁶

$$\sum_{n=-\infty}^{\infty} J_{n+m}(X) J_{n+q}(X) = \delta_{mq},$$

$$\begin{aligned} \sum_{n=-\infty}^{\infty} n J_{n+m}(X) J_{n+q}(X) \\ = -m \delta_{mq} + \frac{X}{2} (\delta_{m(q+1)} + \delta_{m(q-1)}), \end{aligned}$$

$$\begin{aligned} \sum_{n=-\infty}^{\infty} n^2 J_{n+m}(X) J_{n+q}(X) \\ = \left(m^2 + \frac{X^2}{2} \right) \delta_{mq} - X ([m-0.5] \delta_{m(q+1)} \\ + [m+0.5] \delta_{m(q-1)}) + \frac{X^2}{4} (\delta_{m(q+2)} + \delta_{m(q-2)}). \end{aligned} \quad (24)$$

After that, substituting Eq. (17) and applying the inverse Fourier transformation, Eq. (14b), we sum over q and m . Finally, we represent the dc current I_α flowing in lead α under the action of an oscillating scatterer and oscillating reservoir potentials in the following way:

$$I_\alpha = \int_0^\infty dE \left(-\frac{\partial f_0(E)}{\partial E} \right) \{ I_\alpha^{(pump)} + I_\alpha^{(rect)} + I_\alpha^{(int)} \}, \quad (25a)$$

$$I_\alpha^{(pump)}(E) = i \frac{e}{2\pi} \left(\frac{\partial \hat{S}_0(E, t)}{\partial t} \hat{S}_0^\dagger(E, t) \right)_{\alpha\alpha}, \quad (25b)$$

$$I_\alpha^{(rect)}(E) = G_0 \sum_\beta \overline{[V_\beta(t) - V_\alpha(t)] |S_{0,\alpha\beta}(E, t)|^2}, \quad (25c)$$

$$\begin{aligned} I_\alpha^{(int)}(E) \\ = \frac{G_0}{2} \sum_\beta \overline{V_\beta(t) (4\hbar\omega \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] + \mathcal{P}\{S_{0,\alpha\beta}; S_{0,\alpha\beta}^*\})}. \end{aligned} \quad (25d)$$

Here the bar denotes the time average $\bar{X} = (1/T) \int_0^T dt X(t)$ over a time period $T = 2\pi/\omega$; $G_0 = e^2/h$ is the spinless conductance quantum; the function $\mathcal{P}\{X; Y\}$ is defined in Eq. (21b). To arrive at Eq. (25c) we used the unitarity condition $\sum_\beta |S_{0,\alpha\beta}|^2 = 1$ and the fact that the average potential is zero: $\overline{V_\alpha(t)} = 0$.

We emphasize that in the above expressions we omitted all the terms which are of the second (and higher) order in frequency ω and/or in potentials V_α . Next we characterize briefly the three contributions to the current I_α .

The current $I_\alpha^{(pump)}$ is due to solely the oscillating scatterer. It determines the quantum pump effect when the reservoirs are stationary. It is the formula obtained by Brouwer.¹³

The current $I_\alpha^{(rect)}$ is a consequence of the rectification of ac currents flowing in the system under the influence of ac potentials V_α applied to the reservoirs. In context of pumping this effect was considered by Brouwer in Ref. 47. Note that this rectified current depends on the conductances $G_{\alpha\beta} = -G_0 |S_{\alpha\beta}|^2$ and the corresponding potential differences $\Delta V_{\alpha\beta}(t) = V_\beta(t) - V_\alpha(t)$ in close analogy with the dc current flowing in response to a dc voltage. We stress that here $\Delta V_{\alpha\beta}(t)$ depends not only on the amplitudes of the corresponding potentials but also on the phase lag $\Delta\varphi_{\alpha\beta} = \varphi_\alpha$

$-\varphi_\beta$ as well. In particular, if the amplitudes of two oscillating potentials are equal ($V_\alpha = V_\beta = V_0$) then the potential difference reads

$$\Delta V_{\alpha\beta}(t) = 2V_0 \sin\left(\frac{\varphi_\alpha - \varphi_\beta}{2}\right) \sin\left(\omega t + \frac{\varphi_\alpha + \varphi_\beta}{2}\right). \quad (26)$$

This equation [together with Eq. (25c)] shows clearly that the rectification of ac currents can depend on the phase lag between the applied ac potentials and, hence, it can mimic a quantum pump effect.⁴⁷

The third term $I_\alpha^{(int)}$ is novel. Interestingly, as we will see, this current renormalizes both $I_\alpha^{(pump)}$ and $I_\alpha^{(rect)}$. The current $I_\alpha^{(int)}$ is a consequence of the *interference* between the ac currents produced by the external voltages and the ac currents produced by the nonstationary scatterer. An “oscillating” scatterer is much richer in physics than expressed by Eq. (25c). The expression for $I_\alpha^{(rect)}$ is widely used but this is only a part of a correct answer. The part ($I_\alpha^{(rect)}$) is due to a rectification of external currents caused by the time dependence of the conductances. The oscillating scatterer is much richer. It generates its own ac currents which can interfere with the external ac currents. This interference effect leads to $I_\alpha^{(int)}$.

Note that one can extract the contribution $I_\alpha^{(int)}$ from the experimentally measured current by using its linear dependence in both the pump frequency ω and the amplitude of the external voltages V_β , assuming that the latter can be externally controlled. On the other hand if the voltages V_β are

induced by the time-dependent pump current flowing through an external circuit, then the magnitude of the interference current $I_\alpha^{(int)}$ is determined not only by the intrinsic properties of the pump but also by the circuit's impedance and its frequency dependence. In this case identification of the different contributions to the pump current might be difficult unless the external impedance is well characterized.

Before proceeding we check the current conservation. To this end we sum I_α over the lead index α . Note that each of the currents $I_\alpha^{(pump)}$, $I_\alpha^{(rect)}$, and $I_\alpha^{(int)}$ is separately conserved. This fact supports the current decomposition introduced above.

For the pump currents $I_\alpha^{(pump)}$, using the Birman-Krein formula⁵⁷ we find

$$\sum_\alpha I_\alpha^{(pump)} \sim \text{Tr} \left(\frac{\partial \hat{S}_0}{\partial t} \hat{S}_0^\dagger \right) = \frac{\partial}{\partial t} \overline{\ln(\det \hat{S}_0)} = 0.$$

Here we take into account that the average of a time derivative is identically zero: $\overline{\partial X(t)/\partial t} = 0$; Tr denotes the trace of a matrix: $\text{Tr} \hat{S} = \sum_\alpha S_{\alpha\alpha}$.

The conservation of the rectification currents $\sum_\alpha I_\alpha^{(rect)} = G_0 \sum_{\alpha,\beta} \overline{[V_\beta(t) - V_\alpha(t)] |S_{0,\alpha\beta}|^2} = 0$ follows from the unitarity condition $\sum_\alpha |S_{0,\alpha\beta}|^2 = \sum_\beta |S_{0,\alpha\beta}|^2 = 1$.

The current $I_\alpha^{(int)}$ is conserved as well. Since the matrix $\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}$ [Eq. (21b)], is traceless, we get from Eqs. (25d) and (22b) the following:

$$\sum_{\alpha=1}^{N_r} I_\alpha^{(int)} = \frac{G_0}{2} \sum_\beta V_\beta(t) \sum_{\alpha=1}^{N_r} (4\hbar \omega \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] + \mathcal{P}\{S_{0,\alpha\beta}; S_{0,\alpha\beta}^*\}) = \frac{G_0}{2} \sum_\beta V_\beta(t) (\overline{\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}_{\beta\beta}} - \overline{\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}_{\beta\beta}}) = 0.$$

To shed more insight onto the nature of the new contribution $I_\alpha^{(int)}$ we consider a simple but a quite generic example.

A. Two terminal single-channel scatterer

Consider a nonstationary scatterer connected to only two reservoirs $\alpha=1,2$ via single-channel leads. For such a scatterer, assuming there are no magnetic fields, the stationary scattering matrix \hat{S}_0 is a symmetric 2×2 unitary matrix.

$$\hat{S}_0 = e^{i\gamma} \begin{pmatrix} \sqrt{R} e^{-i\theta} & i\sqrt{T} \\ i\sqrt{T} & \sqrt{R} e^{i\theta} \end{pmatrix}. \quad (27)$$

Here R and T are the reflection and the transmission probability, respectively ($R+T=1$). The phase θ characterizes the asymmetry between the reflection to the left and to the right. The phase γ relates to the change of the overall charge δQ on the scatterer (for instance, a dot) via the Friedel sum rule:⁵⁸ $\delta\gamma = \pi \delta Q/e$ (where e is the electron charge), or in different notation $\delta Q = e/(2\pi i) \delta[\ln \det \hat{S}]$. We assume that

$R, T = 1 - R, \theta, \gamma$ are functions of the electron energy E and the external parameters $P_i(t)$ varying with frequency ω . Before proceeding we remark that for the symmetric-in-lead indices case with $N_r=2$ the current $I_\alpha^{(int)}$ [Eq. (25d)] can be simplified. Substituting Eq. (22a) in Eq. (25d) we get

$$I_\alpha^{(int)} = \frac{G_0}{2} \overline{(V_\beta(t) \mathcal{P}\{S_{0,\beta\beta}^*; S_{0,\beta\beta}\} - V_\alpha(t) \mathcal{P}\{S_{0,\alpha\alpha}^*; S_{0,\alpha\alpha}\})}, \quad \alpha \neq \beta. \quad (28)$$

Substituting the scattering matrix [Eq. (27)] into Eqs. (25) and (28) we find the currents $I_1 = -I_2$ flowing between the scatterer and the reservoirs:

$$I_1^{(pump)}(E) = \frac{e}{2\pi} R(E, t) \frac{\partial \theta(E, t)}{\partial t}, \quad (29a)$$

$$I_1^{(rect)}(E) = G_0 \overline{T(E, t) [V_2(t) - V_1(t)]}, \quad (29b)$$

$$\begin{aligned}
 I_1^{(int)}(E) = & \frac{e^2}{4\pi} \overline{\left(\frac{\partial \theta}{\partial t} \frac{\partial R}{\partial E} - \frac{\partial \theta}{\partial E} \frac{\partial R}{\partial t} \right)} [V_2(t) + V_1(t)] \\
 & + \frac{e^2}{4\pi} \overline{\left(\frac{\partial \gamma}{\partial t} \frac{\partial R}{\partial E} - \frac{\partial \gamma}{\partial E} \frac{\partial R}{\partial t} \right)} [V_2(t) - V_1(t)].
 \end{aligned} \tag{29c}$$

These expressions demonstrate that the current $I^{(int)}$ has common features with both the rectification current $I^{(rect)}$ and the pumped current $I^{(pump)}$. Like the former, the current $I^{(int)}$ depends on the potential difference ΔV_{12} . Like the latter, the current $I^{(int)}$ can exist even at equal reservoir potentials $V_1(t) = V_2(t)$. In this case, the conditions necessary for the existence of $I^{(int)}$ and $I^{(pump)}$ are the same:³⁰ First, the scatterer has to be asymmetric, i.e., $\theta \neq 0$, and, second, the time-reversal symmetry (TRS) has to be broken. We note that the current $I^{(int)}$ depends on both the oscillating reservoir potentials $V_\alpha(t) = V_\alpha \cos(\omega t + \varphi_\alpha)$ and the oscillating scattering parameters $P_i(t) = P_{i,0} + P_{i,1} \cos(\omega t + \phi_i)$. Therefore analyzing the presence/absence of the TRS we have to consider all the phases, namely φ_α as well as ϕ_i .

We have here treated only noninteracting electrons. As a consequence, sums of potentials appear in Eq. (29c). This is in contrast with an electrically self-consistent theory which permits only the appearance of voltage differences. If interactions are switched on¹ then the (self-consistent) potential $U \neq 0$ inside the scatterer becomes dependent on external potentials V_α , and the differences $V_\alpha - U$ should appear instead of V_α . U is in general a function of all the oscillating parameters $P_i(t)$, all the external potentials V_α and also of the potentials at the gates which influence the electrostatic potential inside the scatterer. Our expressions do, however, conserve current.

We see that the first term on the RHS of Eq. (29c) renormalizes the pumped current $I_1^{(pump)}$ and the second one renormalizes the rectification current $I_1^{(rect)}$. The latter is due to nonadiabatic (first order in ω) corrections to the conductances arising from the corresponding corrections [Eq. (17)] to the scattering matrix. Note that the analogous corrections are discussed in Refs. 25 and 46 in context of pumping in the presence of a dc bias.

Since the pump effect is the main topic of this work we consider now the case with $V_1(t) = V_2(t)$ in more detail. This case corresponds to an experimental setup in which the scatterer and a large portion of the reservoirs to which it is connected are subject to long-wavelength radiation. The effect of such radiation can be modeled via an oscillating uniform potential $V(t)$ which is the same at different reservoirs: $V_1(t) = V_2(t) \equiv V(t)$. In this case the rectification current [Eq. (29b)] is absent, $I_1^{(rect)} = 0$, and the whole dc current I_1 can be reduced to the simple form

$$I_1 = \frac{e}{2\pi} \int_0^\infty dE \left(- \frac{\partial f_0(E)}{\partial E} \right) \overline{R(\mathcal{E}, t) \frac{d\theta(\mathcal{E}, t)}{dt}}, \quad \mathcal{E} = E + eV(t). \tag{30}$$

To obtain this result we have used the following identity: $-A(\partial R/\partial t) = R(\partial A/\partial t)$ with $A = eV(\partial\theta/\partial E)$. We have also

introduced the full time derivative: $d/dt = (\partial/\partial t) + e(dV/dt)(\partial/\partial \mathcal{E})$.

This result can be understood in the following way: For stationary reservoirs [$V(t) = 0$] the pumped current is described by Eqs. (25a) and (29a) with the quantities R and θ taken at the energy E of incident electrons. However, if the chemical potential $\mu(t) = \mu_0 + eV(t)$, $V(t) \neq 0$ oscillates slowly ($\omega \rightarrow 0$), then we can consider incident electrons having energy $\mathcal{E} = E + eV(t)$ following adiabatically the reservoir's potential $V(t)$. Substituting in Eq. (29a) \mathcal{E} instead of E and replacing a partial time derivative by a full time derivative we get Eq. (30).

It should be noted that the above substitution $\mathcal{E} = E + eV(t)$ implies that the potential inside the scatterer ($U = 0$) is independent of the external potentials V_α . This is correct for noninteracting electrons but it should be modified if the interactions are present.¹

From Eq. (30) we can conclude that the effect of an oscillating external potential $V(t)$ is like the effect generated by an oscillating parameter of the scatterer (i.e., an oscillating internal potential). Therefore to analyze the ability of an open system (the scatterer plus reservoirs) to generate adiabatic dc currents we have to consider the full set of oscillating parameters $\{V_\alpha(t), P_i(t)\}$ ($\alpha = 1, 2, \dots, N_r; i = 1, 2, \dots, N_p$).

On the other hand external voltages cannot be entirely viewed as mere pump (i.e., internal) parameters. External voltages affect the incoming carriers whereas the pump parameters affect only outgoing carriers.

V. DC CURRENT AT FINITE AC VOLTAGES

Now we go beyond linear-response theory. We suppose that the potentials V_α can be large compared to the temperature. Thus we calculate the current [Eq. (12)] with accuracy up to the first order in ω and with an arbitrary ratio of the potentials V_α to the temperature:

$$\hbar \omega \ll k_B T_0, \tag{31a}$$

$$eV_\alpha \ll \mu_{0,\alpha}. \tag{31b}$$

Since the potentials V_α are not necessarily small compared to the temperature T we cannot expand the Fermi function $f_{0,\beta}(E - n\hbar\omega)$ entering Eq. (12). Nevertheless, Eq. (31a) allows us to sum over n and to simplify Eq. (12).

To this end we go from the energy representation over to the time representation. We express the Fermi function $f_{0,\beta}(E)$, Eq. (5), and the Bessel functions $J_n(x)$ as follows:

$$f_{0,\beta}(E - n\hbar\omega) = \int_{-\infty}^{\infty} d\tau f_{0,\beta}(\tau) e^{i(E - n\hbar\omega)(\tau/\hbar)},$$

$$J_{n+q} \left(\frac{eV_\beta}{\hbar\omega} \right) e^{i\varphi_\beta(n+q)} = \frac{1}{T} \int_0^T dt W_\beta^*(t) e^{-i(n+q)\omega t},$$

$$J_{n+m} \left(\frac{eV_\beta}{\hbar\omega} \right) e^{-i\varphi_\beta(n+m)} = \frac{1}{T} \int_0^T dt_1 W_\beta(t_1) e^{i(n+m)\omega t_1},$$

$$f_{0,\beta}(\tau) = \frac{ik_B T_0}{2\hbar \sinh\left(\frac{\pi k_B T_0 \tau}{\hbar}\right)} e^{-i\mu_{0,\beta}(\tau/\hbar)},$$

$$W_\beta(t) = e^{-i(eV_\beta/\hbar\omega)\sin(\omega t + \varphi_\beta)}.$$

Substituting these equations into Eq. (12) and summing over n we obtain a delta function $\delta(t_1 - t - \tau)$ which allows us to perform one additional integration. At $\tau > 0$ ($\tau < 0$) we integrate over t_1 (t). This leads to the substitution $t_1 = t + \tau$ ($t = t_1 + |\tau|$). Further we expand $\sin(\omega\tau + \omega t + \varphi_\beta)$ to first order in $\omega\tau$. We can do this because for the relevant $\tau \ll (\hbar/k_B T_0)$ Eq. (31a) gives $\omega\tau \ll 1$. Next we integrate over τ and finally get the dc current as follows:

$$I_\alpha = \frac{e}{h} \int_0^\infty dE \frac{1}{T} \int_0^T dt \left\{ \sum_\beta \sum_{m,q=-\infty}^\infty \times f_0\left(E + (q+m)\frac{\hbar\omega}{2}; \mu_\beta(t)\right) S_{F,\alpha\beta}^*(E, E_q) \times S_{F,\alpha\beta}(E, E_m) e^{i(m-q)\omega t} - f_0(E; \mu_\alpha(t)) \right\}. \quad (32)$$

Here we have introduced the Fermi function with time-dependent chemical potential $\mu_\alpha(t) = \mu_{0,\alpha} + eV_\alpha(t)$ [Eq. (3)]:

$$f_0(E; \mu_\alpha(t)) = \left[1 + \exp\left(\frac{E - \mu_\alpha(t)}{k_B T_0}\right) \right]^{-1}.$$

Note that Eq. (32) is valid both for the adiabatic as well as for the nonadiabatic case. The only restriction is that the frequency has to be small compared with the temperature, Eq. (31a).

Next we use the adiabatic approximation of Sec. III and calculate the current I_α to first order in frequency ω under the conditions of Eq. (13). To this end we substitute Eq. (17) into Eq. (32) and expand the Fermi function in powers of ω . Next we use the inverse Fourier transformation, Eq. (14b), and after a little manipulation (we integrate by parts on energy and dropped the contribution arising from $E=0$; in addition, we exploit the unitarity of the frozen scattering matrix $\sum_\alpha |S_{0,\alpha\beta}(E,t)|^2 = 1$) and find the current

$$I_\alpha = \frac{e}{h} \int_0^\infty dE \frac{1}{T} \int_0^T dt \left\{ \sum_\beta f_0(E; \mu_\beta(t)) \left[|S_{0,\alpha\beta}(E,t)|^2 + 2\hbar\omega \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] + \frac{1}{2} \mathcal{P}\{S_{0,\alpha\beta}; S_{0,\alpha\beta}^*\} \right] - f_0(E; \mu_\alpha(t)) \right\}. \quad (33)$$

The above equation generalizes Eqs. (25) to the case of finite voltages. Current conservation $\sum_\alpha I_\alpha = 0$ can easily be proven in analogy with Eqs. (25).

Next we concentrate on the pump effect and consider the case with reservoirs having equal oscillating potentials:

$\mu_\alpha(t) \equiv \mu(t) = \mu_0 + eV \cos(\omega t + \varphi)$, $\alpha = 1, \dots, N_r$. Since the Fermi functions entering Eq. (33) become independent of the lead index we can sum up over β and using Eq. (22c) obtain

$$I_\alpha = \int_0^\infty dE \frac{1}{T} \int_0^T dt f_0(E; \mu(t)) \frac{dI_\alpha(E,t)}{dE},$$

$$\frac{dI_\alpha}{dE} = \frac{e}{h} \mathcal{P}\{\hat{S}_0; \hat{S}_0^\dagger\}_{\alpha\alpha} \equiv i \frac{e}{2\pi} \left(\frac{\partial \hat{S}_0}{\partial t} \frac{\partial \hat{S}_0^\dagger}{\partial E} - \frac{\partial \hat{S}_0}{\partial E} \frac{\partial \hat{S}_0^\dagger}{\partial t} \right)_{\alpha\alpha}. \quad (34)$$

The quantity $dI_\alpha(E,t)/dE$ is the spectral current density at energy E and time t (i.e., the current within the energy interval dE) produced by the adiabatically evolving scatterer towards the reservoir α . This definition seems reasonable because of a conservation law $\sum_\alpha dI_\alpha/dE(E,t) = 0$ which is valid at any energy E and at any time moment t . Note that in the case of stationary reservoirs the same interpretation was given in Ref. 40.

These currents (or more precisely, the ability to produce them) are an intrinsic property of a time-dependent scatterer. This property differentiates between a nonstationary scatterer and a ‘‘frozen’’ one. Note that the Fermi distribution function in Eq. (34) describes the filling of (potentially) existing ‘‘current’’ states of a nonstationary scatterer.

At $V=0$ Eq. (34) reproduces Brouwer’s result, Eq. (25b), and agrees with that obtained in Ref. 40. At small voltages $V \rightarrow 0$ for the scattering matrix [Eq. (27)] we get Eq. (30).

Equation (34) determines the dc current to the first order in ω pumped by the slowly oscillating scatterer between the reservoirs having equal (possibly zero) oscillating potentials $V_\alpha(t) = V(t)$. Formally, in the adiabatic case under consideration the effect of oscillating chemical potentials is only the change of an energy of electrons falling upon the scatterer. However, in fact, the phase φ of an oscillating potential $V(t) = V \cos(\omega t + \varphi)$ is of a great importance because of the following. An adiabatically pumped current $I_\alpha \neq 0$ is generated already if the time-reversal symmetry is broken in the *whole system* including the scatterer and the reservoirs. At $V \neq 0$ analyzing this question we have to take into account a possible phase shift between the potentials of reservoirs and the oscillating parameters $P_i(t) = P_{i,0} + P_{i,1} \cos(\omega t + \phi_i)$ of a scatterer. In particular, even a scatterer with a *single* oscillating parameter can produce an adiabatic dc current if only $\phi_1 \neq \varphi$.

VI. INSTANTANEOUS CURRENT

In this section we derive an expression for the instantaneous current of an adiabatic quantum pump simultaneously subject to oscillating external potentials. We first clarify the physical meaning of the (diagonal elements of the) quantity $\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}$ defining (antisymmetric in lead indices) nonadiabatic corrections, Eqs. (21), to the scattering matrix. From the geometrical point of view⁴⁰ $\mathcal{P}\{\hat{S}_0; \hat{S}_0^\dagger\}$ is a curvature in the time-energy plane. The physical interpretation is

based on Eq. (34). We can consider the quantity $dI_{\alpha}/dE(E,t) = (e/h)\mathcal{P}\{\hat{S}_0; \hat{S}_0^{\dagger}\}_{\alpha\alpha}$ as an instantaneous *spectral current* which is pushed by the oscillating scatterer into the lead α .

A more detailed partitioning of the current follows from Eq. (33). We can say that the scatterer drives the following spectral currents from the lead β into the lead α :

$$\frac{dI_{\alpha\beta}}{dE} = \frac{e}{h} \left(2\hbar\omega \text{Re}[S_{0,\alpha\beta}^* A_{\alpha\beta}] + \frac{1}{2} \mathcal{P}\{S_{0,\alpha\beta}; S_{0,\alpha\beta}^*\} \right). \quad (35)$$

The above spectral currents are subject to the following conservation law: $\sum_{\alpha=1}^{N_r} dI(E,t)_{\alpha\beta}/dE = 0$. This property supports the point of view that these currents arise ‘‘inside’’ the scatterer (they are generated by the nonstationary scatterer) without any external current source. Thus we can consider the pump as a source of currents rather than a source of voltages.⁴⁴

In a general case to calculate $dI_{\alpha\beta}/dE$ one needs to know the matrix \hat{A} which can be found from the solution of a non-stationary problem. However, if the stationary scattering matrix \hat{S}_0 is a symmetric in lead indices 2×2 matrix then we can express $dI_{\alpha\beta}/dE$ solely in terms of the frozen scattering matrix $\hat{S}_0(t)$. Using Eq. (22a) we obtain (for $N_r = 2$).

$$\frac{dI_{\alpha\beta}}{dE} = \frac{e}{h} \frac{\mathcal{P}\{\hat{S}_0; \hat{S}_0^{\dagger}\}_{\alpha\alpha} - \mathcal{P}\{\hat{S}_0; \hat{S}_0^{\dagger}\}_{\beta\beta} + 2\mathcal{P}\{S_{0,\alpha\beta}; S_{0,\alpha\beta}^*\}}{4}.$$

In particular, for a scatterer with scattering matrix [Eq. (27)], we obtain the spectral currents as follows:

$$\frac{dI_{11}(E,t)}{dE} = -\frac{e}{4\pi} \left(\frac{\partial(\gamma-\theta)}{\partial t} \frac{\partial R}{\partial E} - \frac{\partial(\gamma-\theta)}{\partial E} \frac{\partial R}{\partial t} \right), \quad (36a)$$

$$\frac{dI_{22}(E,t)}{dE} = -\frac{e}{4\pi} \left(\frac{\partial(\gamma+\theta)}{\partial t} \frac{\partial R}{\partial E} - \frac{\partial(\gamma+\theta)}{\partial E} \frac{\partial R}{\partial t} \right). \quad (36b)$$

The other currents are $dI_{12}/dE = -dI_{22}/dE$ and $dI_{21}/dE = -dI_{11}/dE$. Note that all above currents depend on the phase γ related to the charge of a scatterer.

Strictly speaking, if we are dealing with time-dependent currents (instead of only the time-averaged currents) then we need to show that these currents satisfy the continuity equation for the charge currents:

$$\sum_{\alpha} I_{\alpha}(t) + \frac{\partial Q(t)}{\partial t} = 0. \quad (37)$$

Here $I_{\alpha}(t)$ is the full time-dependent current flowing through the scatterer to the lead α ; $Q(t)$ is the charge of a scatterer.

To calculate $I_{\alpha}(t)$ we first calculate the Fourier transformed current $I_{\alpha,l} = (\omega/2\pi) \int_0^T dt e^{i\omega t} I_{\alpha}(t)$, which reads⁵²

$$I_{\alpha,l} = \frac{e}{h} \int_0^{\infty} dE \{ \langle \hat{b}_{\alpha}^{\dagger}(E) \hat{b}_{\alpha}(E + l\hbar\omega) \rangle - \langle \hat{a}_{\alpha}^{\dagger}(E) \hat{a}_{\alpha}(E + l\hbar\omega) \rangle \}.$$

The operators \hat{b}_{α} and \hat{a}_{α} are defined in Eqs. (8) and (9), respectively. The calculations analogous to those leading to Eq. (33) give us $I_{\alpha,l}$. Performing the inverse Fourier transformation [Eq. (14b)] we finally get the time-dependent current $I_{\alpha}(t)$ flowing in the system as follows:

$$I_{\alpha}(t) = \int_0^{\infty} dE \sum_{\beta} \left\{ \frac{e}{h} [f_0(E; \mu_{\beta}(t)) - f_0(E; \mu_{\alpha}(t))] |S_{0,\alpha\beta}(E,t)|^2 - e \frac{\partial}{\partial t} \left[f_0(E; \mu_{\beta}(t)) \frac{dN_{\alpha\beta}(E,t)}{dE} \right] + f_0(E; \mu_{\beta}(t)) \frac{dI_{\alpha\beta}(E,t)}{dE} \right\}. \quad (38)$$

Here we have introduced the partial density of states¹ for a frozen scatterer,

$$\frac{dN_{\alpha\beta}}{dE} = \frac{i}{4\pi} \left(\frac{\partial S_{0,\alpha\beta}^*}{\partial E} S_{0,\alpha\beta} - S_{0,\alpha\beta}^* \frac{\partial S_{0,\alpha\beta}}{\partial E} \right).$$

These density of states define the charge $Q(t)$ of a frozen scatterer as follows:

$$Q(t) = e \sum_{\alpha} \sum_{\beta} \int_0^{\infty} dE f_0(E; \mu_{\beta}(t)) \frac{dN_{\alpha\beta}(E,t)}{dE}. \quad (39)$$

The quantities $I_{\alpha}(t)$ [Eq. (38)] and $Q(t)$ [Eq. (39)] do satisfy the continuity equation (37).

The three terms in the curly brackets on the RHS of Eq. (38) can be interpreted as follows. The first term defines the currents flowing under the action of external voltages through a frozen scatterer. The second one defines currents attributed to the oscillating charge of a frozen scatterer. The third term can neither be entirely viewed just as a nonadiabatic correction of either the frozen conductance, nor of the frozen density of states. It is more natural to consider it as the ac currents generated by the oscillating scatterer. The ability to generate these ac currents differentiates a nonstationary dynamical scatterer from a merely frozen scatterer.

VII. DISCUSSION

We have investigated the nonstationary adiabatic charge transport through a time-dependent mesoscopic scatterer coupled to reservoirs subject to oscillating voltages. The external voltages applied to the reservoirs induce ac currents flowing through the scatterer. In addition, the oscillating scatterer itself is a source of ac currents flowing between the reservoirs. In general these two types of currents interfere with themselves. This gives rise to a renormalization of the

rectification (i.e., proportional to the potential difference) contribution to the dc current and gives rise to a renormalization of the quantum pump current.

To analyze this interference effect we calculated the Floquet scattering matrix beyond the adiabatic approximation. We investigated the first order in ω corrections to the (adiabatic) scattering matrix and found that the dc currents of both the zeroth and the first order in ω can be expressed in terms of a stationary scattering matrix with time-dependent parameters. Within this approximation, within a noninteracting theory, the oscillating potentials $V_\alpha(t)$ of reservoirs can be accounted for by allowing the energy E of incident particles to follow adiabatically the reservoir potential: $E \rightarrow \mathcal{E} = E + eV_\alpha(t)$.

We emphasize the importance of the phases of all the cyclically evolving quantities (the potentials of reservoirs and the parameters of a scatterer) for generating a dc current. In particular, even when all the reservoirs have the same oscillating potential $V_\alpha(t) = V(t)$ and the rectification effect is ineffective, the dc currents at $V=0$ and at $V \neq 0$ can nevertheless differ significantly.

The analysis allows us to perform a current partition that clarifies the physical meaning of the (diagonal elements of the) quantity $\mathcal{P}\{\hat{S}_0, \hat{S}_0^\dagger\}$ and shows that they correspond to spectral current densities generated by a dynamic scatterer. The instantaneous current contains a contribution from such self-generated ac currents in addition to the currents from the frozen charge and the ac currents generated by the external potentials.

We emphasize that the results presented in this work, the effect of external ac potentials on a quantum pump, are of importance whenever the pump is not part of an ideal zero-impedance external circuit. In particular, if the pump is in series with a resistance used to measure the voltage generated by the pump, or if the circuit is a multiterminal circuit with probes used to measure voltages, the results presented here will be needed.

ACKNOWLEDGMENT

This work was supported by the Swiss National Science Foundation.

APPENDIX

1. The matrix \hat{A}

The matrix \hat{A} defines the first order in frequency corrections to the adiabatic Floquet scattering matrix, Eqs. (17) and (20). If the matrix \hat{S}_0 is symmetric in lead indices then the matrix \hat{A} is antisymmetric in lead indices.

To obtain Eq. (21) we substitute the adiabatic expansion, Eq. (17a), in the current conservation condition, Eq. (16a). Keeping terms of order ω^0 and ω^1 , we get the following:

$$\begin{aligned}
& \sum_\alpha \sum_{n=-\infty}^{\infty} S_{F,\alpha\beta}^*(E_n, E) S_{F,\alpha\gamma}(E_n, E_m) \\
& \approx \sum_\alpha \sum_n \left(S_{0,\alpha\beta,n}^*(E) + \hbar\omega \frac{n}{2} \frac{\partial S_{0,\alpha\beta,n}^*(E)}{\partial E} \right. \\
& \quad \left. + \hbar\omega A_{\alpha\beta,n}^*(E) \right) \\
& \quad \times \left(S_{0,\alpha\gamma,n-m}(E) + \hbar\omega \frac{n+m}{2} \frac{\partial S_{0,\alpha\gamma,n-m}(E)}{\partial E} \right. \\
& \quad \left. + \hbar\omega A_{\alpha\gamma,n-m}(E) \right) \\
& \approx \sum_\alpha \sum_n S_{0,\alpha\beta,n}^*(E) S_{0,\alpha\gamma,n-m}(E) + \sum_\alpha \sum_n S_{0,\alpha\beta,n}^*(E) \\
& \quad \times \left(\hbar\omega \frac{n+m}{2} \frac{\partial S_{0,\alpha\gamma,n-m}(E)}{\partial E} + \hbar\omega A_{\alpha\gamma,n-m}(E) \right) \\
& \quad + \sum_\alpha \sum_n \left(\hbar\omega \frac{n}{2} \frac{\partial S_{0,\alpha\beta,n}^*(E)}{\partial E} \right. \\
& \quad \left. + \hbar\omega A_{\alpha\beta,n}^*(E) \right) S_{0,\alpha\gamma,n-m}(E) \\
& = \delta_{m0} \delta_{\beta\gamma}.
\end{aligned}$$

Applying the inverse Fourier transformation [Eq. (14b)] and introducing corresponding matrixes we rewrite above equation as follows:

$$\begin{aligned}
& \left(|\hat{S}_0(E, t)|^2 + \hbar\omega \hat{S}_0^\dagger(E, t) \hat{A}(E, t) + \hbar\omega \hat{A}^\dagger(E, t) \hat{S}_0(E, t) \right. \\
& \quad \left. + \frac{i\hbar}{2} \hat{S}_0^\dagger \frac{\partial^2 \hat{S}_0}{\partial E \partial t} - i\hbar \frac{\partial}{\partial t} \left[\hat{S}_0^\dagger \frac{\partial \hat{S}_0}{\partial E} \right] - \frac{i\hbar}{2} \frac{\partial^2 \hat{S}_0^\dagger}{\partial E \partial t} \hat{S}_0 \right)_{\beta\gamma, -m} \\
& = \delta_{m0} \delta_{\beta\gamma}. \tag{A1}
\end{aligned}$$

To simplify this equation further we use the unitarity condition for the frozen scattering matrix: $\hat{S}_0(E, t) \hat{S}_0^\dagger(E, t) = \hat{I}$. First, from this condition it follows that

$$(|\hat{S}_0(E, t)|^2)_{\beta\gamma, -m} = \delta_{m0} \delta_{\beta\gamma}. \tag{A2}$$

And second, we can write $(\partial^2 / \partial E \partial t) [\hat{S}_0^\dagger \hat{S}_0] = 0$ and, correspondingly,

$$-\frac{\partial^2 \hat{S}_0^\dagger}{\partial E \partial t} \hat{S}_0 - \hat{S}_0^\dagger \frac{\partial^2 \hat{S}_0}{\partial E \partial t} = \frac{\partial \hat{S}_0^\dagger}{\partial E} \frac{\partial \hat{S}_0}{\partial t} + \frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E}. \tag{A3}$$

Substituting Eqs. (A2) and (A3) in Eq. (A1) we arrive at Eq. (21).

Note that if we use Eq. (16b) instead of Eq. (16a) then we get the condition which is a linear transformation of Eq. (21a) (the LHS and the RHS of Eq. (21a) are multiplied from the left by \hat{S}_0 and from the right by \hat{S}_0^\dagger).

2. The commutator matrix \mathcal{P}

The matrix $\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}$ defined in Eq. (21b) is self-adjoint,

$$\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\} = \mathcal{P}^\dagger\{\hat{S}_0^\dagger; \hat{S}_0\}, \quad (\text{A4})$$

and traceless,

$$\text{Tr}[\mathcal{P}\{\hat{S}_0^\dagger; \hat{S}_0\}] = 0. \quad (\text{A5})$$

To demonstrate the latter property we use the equality $d[\hat{S}]\hat{S}^\dagger = -\hat{S}d[\hat{S}^\dagger]$ following from the unitarity of the scattering matrix $\hat{S}\hat{S}^\dagger = \hat{I}$ and the invariance of trace to the cyclic rearrangements of the matrices. As a result, from Eq. (21b) we get

$$\begin{aligned} \text{Tr}[\mathcal{P}] &= i\hbar \text{Tr} \left[\frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E} - \frac{\partial \hat{S}_0^\dagger}{\partial E} \hat{S} \hat{S}_0^\dagger \frac{\partial \hat{S}_0}{\partial t} \right] \\ &= i\hbar \text{Tr} \left[\frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E} - S^\dagger \frac{\partial \hat{S}_0}{\partial E} \frac{\partial \hat{S}_0^\dagger}{\partial t} \hat{S} \right] \\ &= i\hbar \text{Tr} \left[\frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E} - \frac{\partial \hat{S}_0^\dagger}{\partial t} \frac{\partial \hat{S}_0}{\partial E} \right] = 0. \end{aligned}$$

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- ¹M. Büttiker, H. Thomas, and A. Prêtre, *Z. Phys. B: Condens. Matter* **94**, 133 (1994); M. Büttiker, *J. Phys.: Condens. Matter* **5**, 9361 (1993).
- ²J.B. Pieper and J.C. Price, *Phys. Rev. Lett.* **72**, 3586 (1994).
- ³P.K. Tien and J.P. Gordon, *Phys. Rev.* **129**, 647 (1963).
- ⁴R. Tsu and L. Esaki, *Appl. Phys. Lett.* **22**, 562 (1973).
- ⁵L.P. Kouwenhoven, S. Jauhar, J. Orenstein, P.L. McEuen, Y. Nagamune, J. Motohisa, and H. Sakaki, *Phys. Rev. Lett.* **73**, 3443 (1994).
- ⁶R.H. Blick, R.J. Haug, D.W. van der Weide, K. von Klitzing, and K. Eberl, *Appl. Phys. Lett.* **67**, 3924 (1995).
- ⁷M. Switkes, C.M. Marcus, K. Campman, and A.C. Gossard, *Science* **283**, 1905 (1999).
- ⁸R.G. Mani, J.H. Smet, K. von Klitzing, V. Narayanamurti, W.B. Johnson, and V. Umansky, *Nature (London)* **420**, 646 (2002).
- ⁹M.A. Zudov, R.R. Du, L.N. Pfeiffer, and K.W. West, *Phys. Rev. Lett.* **90**, 046807 (2003).
- ¹⁰L.-H. Reydellet, P. Roche, D.C. Glattli, B. Etienne, and Y. Jin, *Phys. Rev. Lett.* **90**, 176803 (2003).
- ¹¹S.K. Watson, R.M. Potok, C.M. Marcus, and V. Umansky, *Phys. Rev. Lett.* **91**, 258301 (2003).
- ¹²L. DiCarlo, C.M. Marcus, and J.S. Harris, *Phys. Rev. Lett.* **91**, 246804 (2003).
- ¹³P.W. Brouwer, *Phys. Rev. B* **58**, R10 135 (1998).
- ¹⁴I.L. Aleiner and A.V. Andreev, *Phys. Rev. Lett.* **81**, 1286 (1998).
- ¹⁵F. Zhou, B. Spivak, and B. Altshuler, *Phys. Rev. Lett.* **82**, 608 (1999).
- ¹⁶M. Wagner and F. Sols, *Phys. Rev. Lett.* **83**, 4377 (1999).
- ¹⁷A. Andreev and A. Kamenev, *Phys. Rev. Lett.* **85**, 1294 (2000).
- ¹⁸T.A. Shutenko, I.L. Aleiner, and B.L. Altshuler, *Phys. Rev. B* **61**, 10 366 (2000).
- ¹⁹Y. Wei, J. Wang, and H. Guo, *Phys. Rev. B* **62**, 9947 (2000).
- ²⁰J.E. Avron, A. Elgart, G.M. Graf, and L. Sadun, *Phys. Rev. B* **62**, 10 618 (2000).
- ²¹M.G. Vavilov, V. Ambegaokar, and I.L. Aleiner, *Phys. Rev. B* **63**, 195313 (2001).
- ²²J.E. Avron, A. Elgart, G.M. Graf, and L. Sadun, *Phys. Rev. Lett.* **87**, 236601 (2001); *J. Math. Phys.* **43**, 3415 (2002).
- ²³C.-S. Tang and C.S. Chu, *Solid State Commun.* **120**, 353 (2001).
- ²⁴S.-L. Zhu and Z.D. Wang, *Phys. Rev. B* **65**, 155313 (2002).
- ²⁵O. Entin-Wohlman, A. Aharony, and Y. Levinson, *Phys. Rev. B* **65**, 195411 (2002).
- ²⁶M. Moskalets and M. Büttiker, *Phys. Rev. B* **66**, 035306 (2002).
- ²⁷B. Wang and J. Wang, *Phys. Rev. B* **66**, 125310 (2002).
- ²⁸S.W. Kim, *Phys. Rev. B* **66**, 235304 (2002).
- ²⁹M.L. Polianski, M.G. Vavilov, and P.W. Brouwer, *Phys. Rev. B* **65**, 245314 (2002).
- ³⁰M. Moskalets and M. Büttiker, *Phys. Rev. B* **66**, 205320 (2002).
- ³¹M.L. Polianski and P.W. Brouwer, *J. Phys. A* **36**, 3215 (2003).
- ³²T. Aono, *Phys. Rev. B* **67**, 155303 (2003).
- ³³V. Gudmundsson, C.-S. Tang, and A. Manolescu, *Phys. Rev. B* **67**, 161301 (2003).
- ³⁴P. Sharma and C. Chamon, *Phys. Rev. B* **68**, 035321 (2003).
- ³⁵M. Moskalets and M. Büttiker, *Phys. Rev. B* **68**, 075303 (2003).
- ³⁶M. Governale, F. Taddei, and R. Fazio, *Phys. Rev. B* **68**, 155324 (2003).
- ³⁷B. Wang, J. Wang, and H. Guo, *Phys. Rev. B* **68**, 155326 (2003).
- ³⁸D. Cohen, *Phys. Rev. B* **68**, 201303 (2003).
- ³⁹H.-Q. Zhou, S.Y. Cho, and R.H. McKenzie, *Phys. Rev. Lett.* **91**, 186803 (2003); H.-Q. Zhou, U. Lundin, S.Y. Cho and R.H. McKenzie, *Phys. Rev. B* **69**, 113308 (2004).
- ⁴⁰J.E. Avron, A. Elgart, G.M. Graf, and L. Sadun, *math-ph/0305049* (unpublished).
- ⁴¹S.W. Chung, C.-S. Tang, C.S. Chu, and C.Y. Chang, *cond-mat/0306194* (unpublished).
- ⁴²M. Blaauboer, *Phys. Rev. B* **68**, 205316 (2003); *cond-mat/0307166* (unpublished).
- ⁴³A. Banerjee, S. Das, and S. Rao, *cond-mat/0307324* (unpublished).
- ⁴⁴M. Rey and F. Sols, *cond-mat/0308257* (unpublished).
- ⁴⁵V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, *cond-mat/0308382* (unpublished).
- ⁴⁶O. Entin-Wohlman, A. Aharony, and V. Kashcheyevs, *cond-mat/0308408* (unpublished).
- ⁴⁷P.W. Brouwer, *Phys. Rev. B* **63**, 121303 (2001).
- ⁴⁸M.L. Polianski and P.W. Brouwer, *Phys. Rev. B* **64**, 075304 (2001).
- ⁴⁹M. Moskalets and M. Büttiker, *Phys. Rev. B* **64**, 201305 (2001).
- ⁵⁰M. Martinez-Mares, C.H. Lewenkopf, and E.R. Mucciolo, *Phys. Rev. B* **69**, 085301 (2004).

⁵¹M. Büttiker, Phys. Rev. Lett. **65**, 2901 (1990).

⁵²M. Büttiker, Phys. Rev. B **46**, 12 485 (1992).

⁵³M.H. Pedersen and M. Büttiker, Phys. Rev. B **58**, 12 993 (1998).

⁵⁴E.P. Wigner, Phys. Rev. **98**, 145 (1955).

⁵⁵F.T. Smith, Phys. Rev. **118**, 349 (1960).

⁵⁶H. Bateman, in *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953).

⁵⁷D.R. Yafaev, *Mathematical Scattering Theory* (AMS, Providence, RI, 1992).

⁵⁸J. Friedel, Philos. Mag. **43**, 153 (1952).