

Floquet scattering theory of quantum pumps

M. Moskalets¹ and M. Büttiker²

¹*Department of Metal and Semiconductor Physics,*

National Technical University "Kharkov Polytechnical Institute", Kharkov, Ukraine

²*Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland*

(February 1, 2008)

We develop the Floquet scattering theory for quantum mechanical pumping in mesoscopic conductors. The nonequilibrium distribution function, the dc charge and heat currents are investigated at arbitrary pumping amplitude and frequency. For mesoscopic samples with discrete spectrum we predict a sign reversal of the pumped current when the pump frequency is equal to the level spacing in the sample. This effect allows to measure the phase of the transmission coefficient through the mesoscopic sample. We discuss the necessary symmetry conditions (both spatial and temporal) for pumping.

PACS: 72.10.-d, 73.23.-b, 73.40.Ei

I. INTRODUCTION

Quantum charge pumping¹⁻²⁷ is presently of considerable interest. An experiment by Switkes et al. 1 demonstrated that a phase coherent mesoscopic system subjected to a cyclic two parameter perturbation can produce a directed current.

Coherent quantum pumping is a consequence of the interference of energetically different traversal paths made possible by an oscillating scatterer. The ratio of the oscillation frequency ω to the inverse time taken for carriers to traverse the sample τ_T^{-1} defines the operational regime of a pump²⁸⁻³⁰. Brouwer² gave an elegant formulation of adiabatic ($\omega \ll \tau_T^{-1}$) quantum pumping that is based on the scattering matrix approach to low frequency ac transport in phase coherent mesoscopic systems developed by Büttiker, Thomas, and Prêtre³. This approach leads naturally to a geometrical description of adiabatic quantum pumping^{2,12-17}. The theory predicts that the charge pumped during a cycle depends on the area enclosed by the path in the scattering matrix parameter space. A less formal but more physical picture of an adiabatic quantum pump appeals to both quantum mechanical interference and photon assisted transport.^{18,23} The same processes are important for a nonadiabatic ($\omega \gg \tau_T^{-1}$) pump^{31-33,18}. These discussions emphasize the energetics of the carrier traversal process.

It is the purpose of this work to develop a theory that permits the description of both adiabatic and nonadiabatic regimes on the same footing and allows a simple physical interpretation. To this end we extend the approach of Ref. 23 to the case of large frequencies and large pumping amplitudes. We apply the Floquet scattering theory³²⁻³⁶ which deals with the scattering matrix dependent on two energies (incident and outgoing). This approach leads to expressions for the quantities of in-

terest in terms of the side bands of particles exiting the pump. The side bands²⁹ correspond to particles which have gained or lost one or several modulation quanta $\hbar\omega$. This approach is complementary to discussions based on the scattering matrix dependent on two times^{15,24,25}

The paper is organized as follows. In Sec.II the general approach to the kinetics of quantum pumps based on the Floquet scattering theory is presented. In Sec.III we apply the general results to the adiabatic case. In Sec.IV we calculate the Floquet scattering matrix for a particular model - an oscillating double barrier potential - and present the results of numerical calculations of the pumped charge and the heat currents in both adiabatic and nonadiabatic regimes. We conclude in Sec.V.

II. GENERAL APPROACH

We consider scattering^{37,38,3} of an incoming flow of electrons with energy E at a scatterer that oscillates in time with frequency ω .

During the interaction with the oscillating scatterer²⁹ electrons can gain or lose energy quanta $\hbar\omega$. Hence the outgoing state is characterized by the set of energies E_n , $n = 0, \pm 1, \pm 2, \dots$,

$$E_n = E + n\hbar\omega. \quad (1)$$

This is a Floquet state.

According to the Floquet theorem the energy ladder Eq.(1) gives the full set of possible energies for outgoing particles (see e.g.,^{32,35}). Thus to describe scattering due to an oscillating scatterer we can use the Floquet scattering matrix \hat{S}_F . The matrix element $S_{F,\alpha\beta}(E_n, E)$ is the quantum mechanical amplitude for an electron with energy E entering the scatterer through lead β to leave the scatterer through lead α having absorbed ($n > 0$) or

emitted ($n < 0$) energy quanta $|n|\hbar\omega$. The Greek letters α, β , number the leads connecting the sample to N_r reservoirs.

We remark that the negative values $E_n < 0$ correspond to bound states near the oscillating scatterer. These states influence scattering into the propagating ($E_n > 0$) states but they do not directly contribute to the current.

Current conservation implies that the submatrix $\hat{S}_F^{(p)}$ of the Floquet scattering matrix (corresponding to propagating modes only) is a unitary matrix

$$\hat{S}_F^{(p)\dagger} \hat{S}_F^{(p)} = \hat{S}_F^{(p)} \hat{S}_F^{(p)\dagger} = \hat{I}. \quad (2)$$

In particular, if a current with flux 1 and energy E enters the scatterer through lead β then current conservation implies

$$\sum_{\alpha} \sum_{E_n > 0} |S_{F,\alpha\beta}(E_n, E)|^2 = 1. \quad (3)$$

Another useful condition follows from the fact that if all incoming propagating ($E_n > 0$) channels are full then each outgoing channel has also to be full:

$$\sum_{\beta} \sum_{E_n > 0} |S_{F,\alpha\beta}(E, E_n)|^2 = 1. \quad (4)$$

Note that usually the Floquet energy E is determined within the interval $0 \leq E < \hbar\omega$. However, for our problem, it is convenient not to reduce the discrete set of E_n to this interval and to keep E as the actual energy of incident (or outgoing) particles.

Because of Eq.(2) we can express the annihilation operator \hat{b} for outgoing particles in the lead α in terms of annihilation operators \hat{a} for incoming particles in leads $\beta = 1, 2, \dots, N_r$ as follows^{38,23}

$$\hat{b}_{\alpha}(E) = \sum_{\beta} \sum_{E_n > 0} S_{F,\alpha\beta}(E, E_n) \hat{a}_{\beta}(E_n). \quad (5)$$

The operators $\hat{a}_{\alpha}(E)$ obey the following anticommutation relations

$$[\hat{a}_{\alpha}^{\dagger}(E), \hat{a}_{\beta}(E')] = \delta_{\alpha\beta} \delta(E - E').$$

Using Eqs.(2) and (5) we see that the operators $\hat{b}_{\alpha}(E)$ obey the same relations.

Note that above expressions correspond to single (transverse) channel leads and spinless electrons. For the case of many-channel leads each lead index (α, β , etc.) includes a transverse channel index and any repeating lead index implies implicitly a summation over all the transverse channels in the lead. Similarly an electron spin can be taken into account.

Now we calculate the distribution function $f_{\alpha}^{(out)}(E)_{\alpha} = \langle \hat{b}_{\alpha}^{\dagger}(E) \hat{b}_{\alpha}(E) \rangle$ for electrons leaving the scatterer through the lead α . Here $\langle \dots \rangle$ means quantum-statistical averaging. Taking into account Eq.(5) we obtain

$$f_{\alpha}^{(out)}(E) = \sum_{\beta} \sum_{E_n > 0} |S_{F,\alpha\beta}(E, E_n)|^2 \times f_{\beta}^{(in)}(E_n). \quad (6)$$

Here $f_{\beta}^{(in)}(E_n) = \langle \hat{a}_{\beta}^{\dagger}(E) \hat{a}_{\beta}(E) \rangle$ is the distribution function for electrons entering the scatterer through lead β .

A. Directed charge currents

Using the distribution function $f_{\alpha}^{(out)}(E)$ for outgoing particles and $f_{\alpha}^{(in)}(E)$ for incoming ones we can find the directed current I_{α} in the lead α far from the scatterer²³

$$I_{\alpha} = \frac{e}{h} \int_0^{\infty} dE \left\{ f_{\alpha}^{(out)}(E) - f_{\alpha}^{(in)}(E) \right\}. \quad (7)$$

The current directed from the scatterer towards the reservoir is positive by definition. Substituting Eq.(6) into the above equation, using Eq.(4), and making the shift $E \rightarrow E - n\hbar\omega$ we find

$$I_{\alpha} = \frac{e}{h} \int_0^{\infty} dE \sum_{\beta} \sum_{E_n > 0} |S_{F,\alpha\beta}(E_n, E)|^2 \times \left(f_{\beta}^{(in)}(E) - f_{\alpha}^{(in)}(E_n) \right). \quad (8)$$

Here $\sum_{E_n > 0}$ means a sum over those n (positive and negative) for which $E_n = E + n\hbar\omega > 0$.

Another useful representation for the directed current can be obtained if we use Eq.(3) and make the shift $E \rightarrow E - n\hbar\omega$ in $f_{\alpha}^{(out)}(E)$ in Eq.(7). As a result we obtain

$$I_{\alpha} = \frac{e}{h} \int_0^{\infty} dE \sum_{\beta \neq \alpha} \sum_{E_n > 0} \left\{ |S_{F,\alpha\beta}(E_n, E)|^2 f_{\beta}^{(in)}(E) - |S_{F,\beta\alpha}(E_n, E)|^2 f_{\alpha}^{(in)}(E) \right\}. \quad (9)$$

From this expression for the directed current it follows that only transmission $\alpha \neq \beta$ (not reflection $\alpha = \beta$) contributes to the current. In addition Eq.(9) can help us to consider the effect of time reversal symmetry (TRS) on the pumped current.

On the one hand, the time reversal $t \rightarrow -t$ (TR) interchanges incoming and outgoing channels

$$[S_{F,\alpha\beta}(E_n, E)]^{(TR)} = S_{F,\beta\alpha}(E, E_n).$$

Hence if the TRS is present then Eq.(9) reads

$$I_\alpha^{(TRS)} = \frac{e}{h} \int_0^\infty dE f_0(E) \sum_{\beta \neq \alpha} \sum_{E_n > 0} \quad (10)$$

$$(|S_{F,\alpha\beta}(E_n, E)|^2 - |S_{F,\alpha\beta}(E, E_n)|^2).$$

In the above equation (in accordance with the usual pump setup) we suppose that incoming electrons in all the channels are described by the same Fermi distribution function with temperature T and electrochemical potential μ :

$$f_\alpha^{(in)}(E) = f_0(E) \equiv \frac{1}{1 + \exp\left(\frac{E-\mu}{k_B T}\right)}.$$

Generally, the Floquet scattering matrix elements for transmission with incident energy E to E_n is not equal to the transmission from E_n to E ,

$$S_{F,\alpha\beta}(E_n, E) \neq S_{F,\alpha\beta}(E, E_n).$$

From this we can conclude that even a pump with TRS can generate a directed current. If these two scattering amplitudes are not equal, there exists the possibility of empty states deep below the Fermi surface^{39,40}. In this case interaction and inelastic effects¹¹ can be expected to be especially important.

However, if the scattering matrix is energy independent on the scale of the order of $\hbar\omega$

$$S_{F,\alpha\beta}(E_n, E) \approx S_{F,\alpha\beta}(E),$$

then the scatterer with TRS can not produce a dc current. The last circumstance is especially important for the adiabatic case $\omega \rightarrow 0$, since the adiabatic scattering matrix Eq.(16) satisfies the above condition.

On the other hand, in general, the nonstationary case is without TRS and the oscillating scatterer can, in principle, generate a current. In particular, if two parameters of the scatterer oscillate in time with the same frequency ω but with phase lag $\Delta\varphi$ then the time reversal implies the reversal of the sign of $\Delta\varphi$. Thus for a pump with $\Delta\varphi \neq 0$ the scattering problem is without TRS (the time reversal symmetry is dynamically broken) and such a scatterer can produce a dc current. This effect was used for generating a dc current in adiabatic quantum pumps¹.

B. Directed heat currents

By analogy with Eq.(7) we find the directed heat current $I_{E,\alpha}$ flowing in lead α away from the scatterer^{41-43,23} (we suppose that all the reservoirs are at the same electrochemical potential μ)

$$I_{E,\alpha} = \frac{1}{h} \int_0^\infty dE (E - \mu) \times \left\{ f_\alpha^{(out)}(E) - f_\alpha^{(in)}(E) \right\}. \quad (11)$$

With the distribution function for outgoing particles $f^{(out)}$ from Eq.(6) we get

$$I_{E,\alpha} = \frac{1}{h} \int_0^\infty dE \sum_\beta \sum_{E_n > 0} (E_n - \mu) \times |S_{F,\alpha\beta}(E_n, E)|^2 \left(f_\beta^{(in)}(E) - f_\alpha^{(in)}(E_n) \right). \quad (12)$$

Note that if all the reservoirs are at the same macroscopic conditions (electrochemical potential, temperature, etc.) then the heat flow $I_{E,\alpha}$ (at any lead $\alpha = 1, 2, \dots, N_r$) is directed from the scatterer to the reservoir²³. That differs strongly from the charge current I_α given by Eq.(8) which, if it exists, can be directed either from the reservoir to the scatterer (at some lead) or vice versa (at another lead).

III. ADIABATIC APPROXIMATION

In this section we use the above formalism to investigate the limit of adiabatic scattering.

The general physical notion of adiabaticity applied to the scattering problem of interest here is as follows: Let us suppose that the time independent problem is described by the scattering matrix $\hat{S}_0(E, X_1, \dots, X_N)$ which depends on the energy E of incident electrons and a set of parameters X_i , $i = 1, 2, \dots, N$. Next assume that the parameters X_i vary in time: $X_i = X_i(t)$. Then we can say that the nonstationary scattering problem is *adiabatic* if scattering of particles incident with energy E can be described via the scattering matrix \hat{S}_0 with time-dependent parameters $X_i(t)$

$$\hat{S}_{ad}(E, t) = \hat{S}_0(E, X_1(t), \dots, X_N(t)). \quad (13)$$

This approximation is adequate if the scattering matrix changes only a little while an electron interacts with the scatterer. In other words, the characteristic time scale for the change of parameters X_i is much larger than the traversal time τ_T .

An analogous criterion can be formulated concerning the energy dependence of the scattering matrix. To this end we consider the adiabatic problem when the parameters change periodically in time: $X_i(t) = X_i(t + 2\pi/\omega)$. In this case we can expand the adiabatic scattering matrix into the Fourier series

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

where

$$\hat{S}_{0,n}(E) = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} dt e^{i\omega t} \quad (15)$$

$$\times \hat{S}_0(E, X_1(t), \dots, X_N(t)).$$

The Fourier harmonics $S_{0,n}$ define the amplitudes of side bands for particles traversing the adiabatically oscillating scatterer with initial incident energy E . Thus we can construct the adiabatic Floquet scattering matrix as follows

$$\hat{S}_{F,ad}(E_n, E) = \hat{S}_{F,ad}(E, E_{-n}) = \hat{S}_{0,n}(E). \quad (16)$$

The adiabatic Floquet scattering matrix consists thus for each incident energy of a block of dimension of $(2N_r n_{max})^2$ where N_r is the number of leads and n_{max} is the maximum number of side bands needed for an accurate description of the quantities of interest.

The above equation allows us to formulate the following adiabaticity criterion: If the Floquet scattering matrix \hat{S}_F changes only a little when the energy E changes by $n_{max}\hbar\omega$ then the adiabatic approximation can be applied and $\hat{S}_F \approx \hat{S}_{F,ad}$. Note that because of Eq.(16) the same criterion can be applied to the scattering matrix $\hat{S}_0(E)$.

Let us now calculate the directed charge current I_{ad} and a heat flow $I_{E,ad}$ in the adiabatic limit. Substituting Eq.(16) into Eq.(8) we find the current flowing in lead α under an adiabatic change of parameters (we put $f^{(in)} = f_0$):

$$I_{ad,\alpha} = \frac{e\omega}{2\pi} \int_0^\infty dE \left(-\frac{\partial f_0(E)}{\partial E} \right) \quad (17)$$

$$\times \sum_\beta \sum_n n |S_{0,\alpha\beta,n}(E)|^2.$$

We see that the current I_{ad} is due to photon-assisted processes (the current depends on the intensity of side bands which is proportional to $|S_{0,\alpha\beta,n}(E)|^2$). Therefore even in the "adiabatic" limit pumping is, strictly speaking, a nonadiabatic phenomenon.

Note that formally Eq. (17) is obtained for $\hbar\omega \ll k_B T$. However it gives the correct answer (in the adiabatic limit) for an arbitrary ratio of the frequency ω to the temperature T .

Using Eq.(14) we can rewrite Eq.(17) as follows

$$I_{ad,\alpha} = i \frac{e\omega}{4\pi^2} \int_0^{2\pi/\omega} dt \int_0^\infty dE \left(-\frac{\partial f_0(E)}{\partial E} \right) \quad (18)$$

$$\times \left(\frac{\partial \hat{S}_0(E,t)}{\partial t} \hat{S}_0^\dagger(E,t) \right)_{\alpha\alpha}.$$

This is Brouwer's formula². We emphasize that Eq.(17) and Eq.(18) express a (nonadiabatic in nature) pumped current in terms of the scattering matrix \hat{S}_0 for a "frozen" scatterer with time-dependent parameters (see Eq.(13)). This is correct if the scattering matrix \hat{S}_0 can be taken

to be energy independent on the scale of the order of $n_{max}\hbar\omega$. The last conclusion is correct irrespective of the amplitude of the oscillating parameters. But n_{max} might very well depend on whether one is in the weak amplitude limit or in the strong amplitude limit.

Next consider the heat flow $I_{E,ad,\alpha}$ produced by the adiabatically oscillating scatterer in the lead α . Substituting the adiabatic scattering matrix Eq.(16). into Eq.(12) we find

$$I_{E,ad,\alpha} = \frac{1}{h} \int_{-\infty}^\infty d\epsilon \sum_\beta \sum_n |S_{0,\alpha\beta,n}(\mu + \epsilon)|^2 \quad (19)$$

$$\times \frac{\left(\epsilon + \frac{n\hbar\omega}{2} \right) \sinh\left(\frac{n\hbar\omega}{2k_B T} \right)}{\cosh\left(\frac{\epsilon}{k_B T} \right) + \cosh\left(\frac{n\hbar\omega}{2k_B T} \right)}.$$

At zero temperature (or if the temperature T is less than the relevant energy scale for the scattering matrix \hat{S}_0) the above equation can be greatly simplified. In this case the heat flow can be expressed in terms of an on-shell, time-dependent adiabatic scattering matrix $\hat{S}_0(\mu, t)$:

$$I_{E,ad,\alpha} = -\frac{\hbar\omega}{8\pi^2} \int_0^{2\pi/\omega} dt \quad (20)$$

$$\times \left(\frac{\partial^2 \hat{S}_0(\mu, t)}{\partial t^2} \hat{S}_0^\dagger(\mu, t) \right)_{\alpha\alpha}.$$

This expression coincides with that given by Avron et al. 13.

In the adiabatic limit it is possible to express the quantities of interest in terms of the stationary scattering matrix. This permits the very general and useful expressions discussed in this paragraph. In contrast, in the non-adiabatic case, the information contained in the stationary scattering matrix is by definition not sufficient. As a consequence, in order to address the non-adiabatic case, we have now to consider a very specific example.

IV. CHARGE AND HEAT FLOWS PRODUCED BY AN OSCILLATING DOUBLE BARRIER

To apply the general formalism of Sec.II beyond the adiabatic approximation we investigate a simple model 4. It is a one-dimensional scatterer consisting of two delta function barriers oscillating with frequency ω and located at $x = -L/2$ and $x = L/2$.

To calculate the Floquet matrix we consider scattering of electrons with energy E coming from $x = -\infty$. The time-dependent Schrödinger equation for an electron wave function $\Psi(x, t)$ reads

$$\begin{aligned}
i\hbar \frac{\partial \Psi(x,t)}{\partial t} &= \hat{H}(x,t)\Psi(x,t), \\
\hat{H}(x,t) &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t), \\
V(x,t) &= V_1(t)\delta(x + \frac{L}{2}) + V_2(t)\delta(x - \frac{L}{2}), \\
V_i(t) &= V_{0i} + 2V_{1i} \cos(\omega t + \varphi_i), i = 1, 2.
\end{aligned} \tag{21}$$

Appendix A gives the exact solution of this model. We now use this solution to calculate the charge current flowing through (as well as the heat current flowing from) the oscillating double barrier potential (see Eq.(21)) connecting two reservoirs with the same temperature $T = 0$ and electrochemical potential μ . We use the units $2m = \hbar = e = 1$. To be definite we consider the current I_1 ($I_{E,1}$) flowing to the left ($x \rightarrow -\infty$). The currents are calculated, using Eq.(8) and Eq.(12) with the Floquet scattering matrix determined as shown in Appendix A. We compare these currents with the adiabatic currents $I_{ad,1}$ and $I_{E,ad,1}$ using the Brouwer formula Eq.(18) and its analog Eq.(20).

For reference we write down the scattering matrix $\hat{S}_0(E)$ which we need to calculate the adiabatic currents:

$$\hat{S}_0 = \frac{e^{ikL}}{\Delta} \begin{pmatrix} \xi + 2\frac{p_2}{k} \sin(kL) & 1 \\ 1 & \xi + 2\frac{p_1}{k} \sin(kL) \end{pmatrix}. \tag{22}$$

Here $k = \sqrt{\frac{2m}{\hbar^2} E}$; $p_j = V_j m / \hbar^2$ ($j = 1, 2$); $\xi = (1 - \Delta)e^{-ikL}$; $\Delta = 1 + \frac{p_1 p_2}{k^2} (e^{2ikL} - 1) + i\frac{p_1 + p_2}{k}$. Of interest is a comparison of the exact Floquet scattering matrix and adiabatic theory in the limit of small and large frequencies. Furthermore, it is interesting to compare the symmetry conditions for pumping for the two theories.

A. Adiabatic limit: $\omega \rightarrow 0$

From our calculations it follows that in the limit of $\omega \rightarrow 0$ the adiabatic current I_{ad} gives a good approximation for the pumped current irrespective of the amplitude of the oscillating potentials V_{1i} . However the criterion of adiabaticity depends strongly on the ratio $V_{1i}/\hbar\omega$.

As we have seen, the adiabatic approximation is valid if the scattering matrix \hat{S}_0 is energy independent on the scale of the order of $n_{max}\hbar\omega$. Here n_{max} (specified below) is the number of side bands with noticeable amplitude excited by the oscillating scatterer. Let us denote by δE the energy scale over which the scattering matrix \hat{S}_0 changes significantly. For example, close to a resonance δE is of the order of the width δ of a resonance. Then the adiabatic approximation is valid if $n_{max}\hbar\omega \ll \delta E$. Hence the larger the number n_{max} of excited side bands the smaller the frequencies for which the adiabatic approximation is valid.

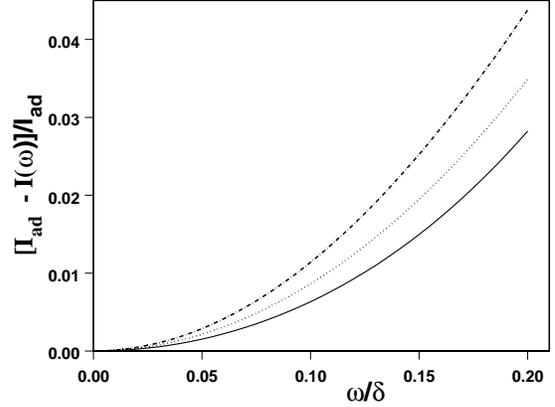


FIG. 1. Relative change of the pumped current $[I_{ad} - I(\omega)]/I_{ad}$ as a function of the pump frequency ω for three values of an oscillating potential $V_{11} = V_{12} = 0.02$ (solid line); 1 (dotted line); and 2 (dash-dotted line) close to the transmission resonance. The frequency is measured in units of the width of the resonance $\delta = 0.339$. The parameters are: $L = 2\pi$; $\mu = 24.167$; $V_{01} = V_{02} = 20$; $\varphi_1 - \varphi_2 = \pi/2$. We use the units: $2m = \hbar = e = 1$.

As it is well known³² the number n_{max} of excited side bands depends on the ratio of the amplitude of the oscillating potential V_{1i} to the frequency ω . In the small amplitude limit $V_{1i} \rightarrow 0$ only the first side bands are excited: $n_{max} = 1$. But for strong pumping the number n_{max} is large and the adiabatic approximation is valid only at smaller frequencies. As a consequence for a given finite frequency ω the deviation of the actual pumped current $I(\omega)$ from the adiabatic one I_{ad} increases with increasing pumping amplitude. This fact is illustrated in Fig.1.

Before concluding this subsection we would like to emphasize the following. For strong pumping the adiabatic approximation is still valid at sufficiently small frequencies despite the excitation of a large number of side bands. The Fourier harmonics of the scattering matrix \hat{S}_0 define the amplitudes of side bands for strong (Eq.(16)) as well as for weak²³ adiabatic pumping. Thus the scattering matrix \hat{S}_0 completely defines the kinetics and, in particular, the quantum statistical correlation properties of an adiabatic pump. The current noise of a weak (small amplitude) pump was considered in Ref. 23. The noise in a strong amplitude adiabatic pump will be presented elsewhere.

B. Large frequency limit

At large frequencies $\omega > \delta$ (where δ is the width of a resonance) the pumped current I differs considerably from the adiabatic one I_{ad} .

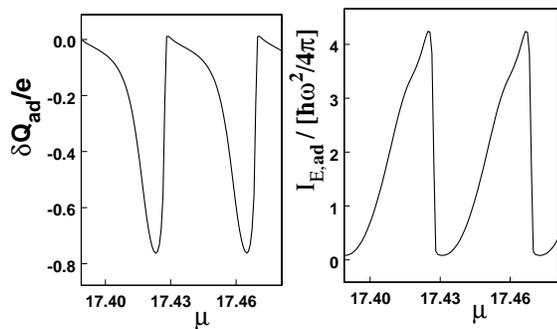


FIG. 2. The adiabatically pumped charge $\delta Q_{ad} = 2\pi I_{ad}/\omega$ (in units of an elementary charge e) during a period (left panel) and the adiabatic heat current $I_{E,ad}$ (in units of $\hbar\omega^2/(4\pi)$) (right panel) as a function of the Fermi energy μ . The parameters are: $L = 200\pi$; $V_{01} = V_{02} = 20$; $V_{11} = V_{12} = 10$; $\varphi_1 - \varphi_2 = \pi/2$.

It is known that for a double barrier structure at $\omega \rightarrow 0$ the pumped dc current I_{ad} ^{8,20} and the generated heat flow $I_{E,ad}$ ²⁵ show a resonance-like behavior as a function of the Fermi energy μ (see Fig.2). The pumped current and heat peak when the Fermi energy is close to the transmission resonance. This is because in the adiabatic limit only the particles close to the Fermi level contribute to the charge (Eq.(18)) and energy (Eq.(20)) transfer.

With increasing pumped frequency $\omega \gg \delta$ the particles within a wider energy interval come into play. The dependence on the Fermi energy is smoothed away. However a resonance-like dependence on the frequency ω arises.

In Fig.3 we depict the dependence of the charge $\delta Q = (2\pi)I/\omega$ pumped during a cycle on the frequency ω . The pumped charge peaks when the energy quantum $\hbar\omega$ equals one (or several) level spacings Δ of a double barrier structure. In the example used for numerical calculations the level spacing Δ near the Fermi energy is constant with good accuracy. The smaller peaks correspond to many ($n = 2, 3, \dots$) photon processes for which $n\hbar\omega = m\Delta$ ($m = 1, 2, \dots$). We see that the single photon processes dominate over the many photon processes.

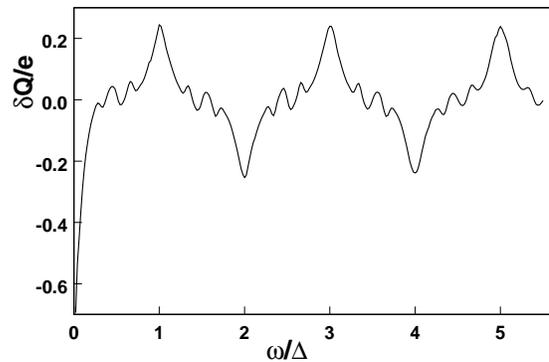


FIG. 3. The charge $\delta Q = 2\pi I/\omega$ pumped during a cycle as a function of the frequency ω (in units of the separation $\Delta = 0.0417$ between the transmission resonances). The Fermi energy is $\mu = 17.423$. The parameters are the same as in Fig.2.

At arbitrary ($n\hbar\omega \neq m\Delta$) but large ($\hbar\omega \gg \delta$) frequencies, due to interference (inside the double barrier structure) only the main component ($n = 0$) of the Floquet state Eq.(23) has a significant amplitude between the barriers. This component corresponds to the eigenfunction of the time independent problem (with barriers V_{01} and V_{02}). The side bands ($n \neq 0$) do not participate in the transmission through the system (more precisely, their contribution is small). As a result the pumped current is greatly reduced compared to the adiabatic case. It should be noted that in the adiabatic case the side bands do contribute to the transmission since for $\omega \ll \delta$ they lie at the same transmission resonance as the main component.

On the other hand at some particular values of a frequency $\hbar\omega = m\Delta$ the substates $\psi_{\pm k}$ ($k = 1, 2, 3, \dots$) of the Floquet state Eq.(23) become large and additional channels for the transmission through the system open up. This leads to the increase of the pumped charge (see main peaks in Fig.3).

Interestingly, as shown in Fig.3), the pumped current reverses sign as a function of frequency. These sign reversals can be understood in the following way: If two potential barriers oscillate then the pump effect arises as a consequence of an interference between two amplitudes¹⁸. The first amplitude \mathcal{A}_1 corresponds to particles which propagate through the double barrier structure and absorb (emit) the energy quantum $\hbar\omega$ (or several quanta $n\hbar\omega$) at the first barrier. The second amplitude \mathcal{A}_2 corresponds to the same propagation with absorption (emission) at the second barrier. As it is known^{1,2} the adiabatically pumped current is an odd function of the phase difference of the oscillating potentials $\Delta\varphi = \varphi_1 - \varphi_2$ (see Eq.(21)). In fact this is the phase difference of the two amplitudes \mathcal{A}_1 and \mathcal{A}_2 . In the nonadiabatic case there exists an additional contribution coming from the spatial

phase difference

$$\Delta\varphi_x \simeq (k_1 - k_2)L.$$

Thus at large frequencies the pumped current depends on the sum $\Delta\varphi + \Delta\varphi_x$.

To clarify the appearance of $\Delta\varphi_x$ let us consider particles with energy E going from the left to the right and absorbing the quantum $\hbar\omega$. The amplitude \mathcal{A}_1 corresponds to particles which absorb an energy $\hbar\omega$ close to the left barrier (V_1) and traverse the system at energy $E + \hbar\omega$. Hence $k_1 \sim \sqrt{E + \hbar\omega}$. On the other hand the amplitude \mathcal{A}_2 corresponds to particles which absorb an energy $\hbar\omega$ close to the right barrier (V_2) and thus traverse the system at energy E . They thus propagate with wave vector $k_2 \sim \sqrt{E}$. Because $k_1 \neq k_2$ there is a phase difference $\Delta\varphi_x$ between the amplitudes \mathcal{A}_1 and \mathcal{A}_2 . Note that in the adiabatic case (i.e., at $\omega \rightarrow 0$) $\Delta\varphi_x$ vanishes.

Now we show that in the case under consideration the phase difference $\Delta\varphi_x$ is at the origin of the sign reversal of the pumped current at consecutive peaks (see Fig.3). Close to the m^{th} main peak of $I(\omega)$ the frequency is determined by $\hbar\omega \sim m\Delta$. Taking into account that only the particles with energy close to the resonance contribute to the transmission and mainly single photon processes are important we can estimate $\Delta\varphi_x$ as follows. If the amplitude \mathcal{A}_1 corresponds to the propagation through some resonance (say E_{l+m}) then \mathcal{A}_2 corresponds to the propagation through the resonance E_l . At the l^{th} transmission resonance it is $k^{(l)}L = l\pi$ the additional phase difference is $\Delta\varphi_x = m\pi$. Thus the sum $\Delta\varphi + \Delta\varphi_x$ changes by π as we pass from one peak to another ($\Delta m = 1$) thus giving rise to the sign reversal⁴⁵.

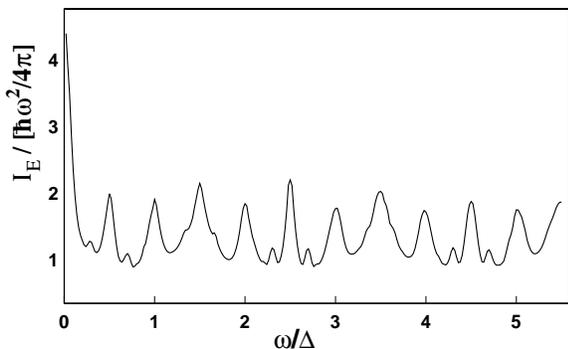


FIG. 4. The heat current I_E (in units of $\hbar\omega^2/(4\pi)$) as a function of the frequency ω . The parameters are the same as in Fig.3.

In addition interference inside the double barrier structure manifests itself as a resonance-like dependence of the heat production (see Fig.4). We can see that $I_E(\omega)$ contains additional peaks at $\hbar\omega = (m + \frac{1}{2})\Delta$. This fact

emphasizes the striking difference between the processes which are responsible for charge pumping and for heat production²³.

C. Quantum pumping and broken symmetry

Our results show that the symmetry of the scattering problem is important for the pump effect.

The quantum pump effect arises due to the different, interfering excitation histories of carriers traversing the sample⁴⁶. To "extract" directed currents from the uniform environment the left-right symmetry (LRS) for carriers traversing the sample needs to be broken. There are, at least, two ways to break the LRS. The first one is breaking the spatial symmetry (SS). The second one is breaking the time reversal symmetry (TRS).

We restrict our considerations to systems which in the absence of the time-dependent perturbations needed for pumping are in an equilibrium state. In particular this means that without the presence of magnetic fields (etc.) the system is time reversal invariant. Note that the time independent scattering problem is insensitive to the presence (absence) of the spatial symmetry of the scatterer (in the sense that the transmission probability is invariant under the spatial inversion $x \rightarrow -x$ irrespectively of the SS of the scattering potential).

Interestingly, the symmetry conditions for pumping depend on the frequency. In the adiabatic limit $\omega \rightarrow 0$ (see Sec.III) the scattering problem is fully characterized by the scattering matrix \hat{S}_0 . In contrast to the conductance, adiabatic pumping is sensitive to the symmetry of the scattering matrix. To have an adiabatic pumping effect we need to break both the spatial symmetry and the time-reversal symmetry.

It is important to distinguish the symmetry of the equilibrium problem and the symmetry of the full problem. In the adiabatic case, the symmetry of the time-independent problem is irrelevant: What matters, is that the system in presence of perturbations breaks both the spatial symmetry and the time reversal symmetry. In many examples (for instance the two barrier problem considered above) it is not possible to break the time-reversal symmetry without at the same time breaking the spatial symmetry. However, examples which are spatially symmetric and have broken time-reversal invariance can be constructed. For instance, we could consider the problem of two barriers oscillating in synchronism and as a second perturbation which oscillates with a phase lag choose the potential between the two barriers. This would be an example of a two parameter problem which does not generate a pumped current. The important point we would like to emphasize is that the symmetry conditions for the non-adiabatic pump are different.

In the strongly nonadiabatic limit the scattering problem is described by the Floquet scattering matrix

$\hat{S}_F(E^{(out)}, E^{(in)})$ dependent on both the incident $E^{(in)}$ and outgoing $E^{(out)}$ energies. In general, the Floquet scattering matrix is sensitive to the spatial symmetry of the scatterer. If the scattering problem is without SS (i.e., when the scattering potential is not invariant under the change $x \rightarrow -x$) then

$$\begin{aligned} & |S_{F,\alpha\beta}(E^{(out)}, E^{(in)})|^2 \\ & \neq |S_{F,\beta\alpha}(E^{(out)}, E^{(in)})|^2, \end{aligned}$$

and the oscillating scatterer can pump a dc current (see Eq.(9)). Thus to obtain a pump effect in the strongly nonadiabatic limit there are, at least, two possibilities. Either the spatial symmetry or the time reversal symmetry (or both SS and TRS together) have to be broken. The role of spatial symmetry breaking for the nonadiabatic pump effect was emphasized in Ref. 18.

The above reasoning is illustrated in Fig.5 where the dependence of a pumped current on the frequency is shown for three generic situations. First, two potentials oscillate with the same amplitude but out of phase (solid line). In this case the perturbation breaks both the spatial symmetry and the time reversal symmetry. Second, only one potential oscillates (dotted line). The TRS is present but the SS is dynamically broken. The system is able to pump a dc current like in the previous case. Third, two potentials oscillate in phase and with the same amplitudes (dash-dotted line). Now both the TRS and SS are preserved and the system under consideration does not exhibit a directed current.

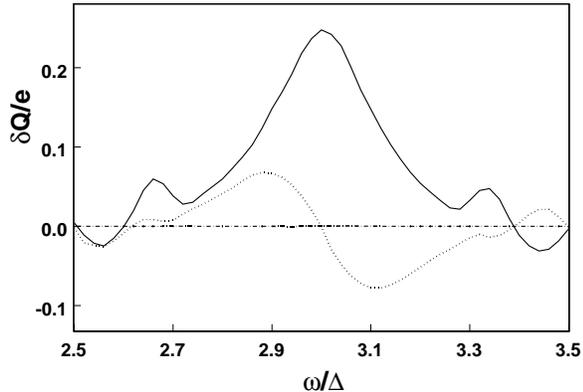


FIG. 5. The charge δQ pumped during a cycle as a function of the frequency ω . Three cases are presented: (i) two potentials $V_{11} = V_{12} = 10$ oscillate out of phase $\varphi_1 - \varphi_2 = \pi/2$ (solid line); (ii) only single potential oscillates: $V_{11} = 10$, $V_{12} = 0$ (dotted line); (iii) two potentials $V_{11} = V_{12} = 10$ oscillate in phase $\varphi_1 = \varphi_2$ (dash-dotted line). The parameters are the same as in Fig.3.

V. DISCUSSION AND CONCLUSION

In this work we have developed the Floquet scattering matrix approach to parametric pumping in phase coherent mesoscopic systems of noninteracting electrons. We have calculated the distribution function, the dc current and the heat flow at arbitrary pumping amplitudes and frequency.

The Floquet scattering matrix describes naturally the existence of the side bands $E_n = E + n\hbar\omega$ of particles leaving the pump. These side bands correspond to nonequilibrium particles generated by the pump which carry the heat from the oscillating scatterer to the reservoirs and (under some conditions) transfer charge between the reservoirs²³. If the pumping amplitude is small only the first ($n = \pm 1$) side bands are excited. But for strong pumping the number of excited side bands is large: $n_{max} \gg 1$. This number together with the frequency defines the energy scale $n_{max}\hbar\omega$ characteristic of the pump problem. In particular this is important for the analysis of the conditions under which the adiabatic approach to pumping is valid. If the scattering matrix is energy independent on the scale of the order of $n_{max}\hbar\omega$ then the adiabatic approximation can be applied. In this case the elements of the Floquet scattering matrix are given by the corresponding Fourier components of the stationary scattering matrix \hat{S}_0 (see Eq.(16)) with parameters taken to be dependent on time.

The existence of the pump effect is directly related to the symmetry of the scattering problem. In the adiabatic case ($\omega \rightarrow 0$) only a scatterer without spatial and time reversal symmetry can produce a directed current. This conclusion applies irrespectively of the (stationary) spatial symmetry of the scatterer. On the other hand in the nonadiabatic case (at large pumping frequency) to achieve pumping we need a scatterer with either broken spatial or time reversal symmetry. Hence at large operating frequencies even the scatterer with a single oscillating parameter can show a pump effect if only the spatial symmetry is broken¹⁸.

To emphasize the main physics underlying pumping we have considered an exactly solvable model. Namely a one-dimensional scatterer consisting of two oscillating delta-function barriers Eq.(21) separated by a distance L .

If two barriers oscillate out of phase (broken TRS) the basic process leading to the pump effect is an interference of two quantum mechanical amplitudes. These amplitudes \mathcal{A}_1 and \mathcal{A}_2 corresponds to particles which traverse the scatterer in the same direction but gain (or lose) a modulation energy in the vicinity either of the first or of the second barrier, respectively¹⁸. This becomes clearer at large frequencies ω because of the following. When the energy quantum $\hbar\omega$ equals one (or several, say m) level spacing Δ of a double barrier structure the pumped current peaks (see Fig.3). The particles with energy close to

the resonance of a double barrier structure give the main contribution to the pump current. Thus the amplitudes \mathcal{A}_1 and \mathcal{A}_2 correspond to traversal of the system through different (say, $(l+m)^{th}$ and l^{th}) resonances. This gives rise to an additional phase difference $\Delta\varphi_x = (k_1 - k_2)L$ between the amplitudes \mathcal{A}_1 and \mathcal{A}_2 . For the resonant double barrier considered here the phase difference between consecutive resonances is π and thus $\Delta\varphi_x = m\pi$. As a result the consecutive peaks of the pumped current have opposite sign (see Fig.3).

We conclude that if the time reversal symmetry is broken (i.e., $\Delta\varphi \neq 0$), the nonadiabatic pumped current contains direct information on the phase of the transmission coefficient through the mesoscopic sample. We emphasize that here we have a single-connected geometry in contrast with the case where the mesoscopic sample (a quantum dot) is embedded in one arm of the ring⁴⁷.

We have also considered the effect of a spatial asymmetry. If only one potential (say, V_1) oscillates then the spatial symmetry is (dynamically) broken. In this case the (nonadiabatic) pump effect arises because the probability for exciting side bands $|S_{F,\alpha\beta}(E_n, E)|^2$ depends on the direction (i.e., on the order of indexes α and β) (see Eq.(9)). The particles going from the left to the right first absorb (emit) the energy $n\hbar\omega = E_n - E$ and then pass through the double barrier structure (at energy E_n). Thus the corresponding probability is

$$|S_{F,21}(E_n, E)|^2 \sim T(E_n).$$

Here $T(E)$ is a transmission probability. On the other hand the particles going from the right to the left pass the system before they absorb (or emit) the energy in the vicinity of the oscillating barrier 1. Hence we have

$$|S_{F,12}(E_n, E)|^2 \sim T(E).$$

Thus the pumped current Eq.(9) depends on the differences $T(E) - T(E \pm n\hbar\omega)$.

Note that for a system with equidistant spectrum (that is the case under consideration) the transmission probability $T(E)$ is periodic in energy E with the period of Δ . Hence if $\hbar\omega = m\Delta$ then it is $T(E) \approx T(E \pm \hbar\omega)$ and the current is close to zero in accordance with Fig.5 (a dotted curve; $m = 3$).

We have presented a scattering theory of quantum pumping based on the Floquet theorem. This approach allows a description of the kinetics of both adiabatic and nonadiabatic quantum pumps. In particular the quantum statistical correlation properties (noise) can be considered in analogy with the weak amplitude adiabatic quantum pump²³. The investigation of noise is especially important in the context of quantized (i.e., noiseless) charge pumping^{13,14,23} and will be presented elsewhere.

ACKNOWLEDGEMENT

This work is supported by the Swiss National Science Foundation.

VI. APPENDIX A: OSCILLATING DOUBLE BARRIER. AN EXACT SOLUTION

In this Appendix we determine the Floquet scattering matrix of the Schrödinger equation (21) of two oscillating delta function potentials located at $x = -L/2$ and $x = L/2$. To find the Floquet matrix we consider scattering of electrons with energy E coming from $x = -\infty$. To solve (21) we use the Floquet functions method⁴⁴. Since the Hamiltonian \hat{H} depends on time, the system has no stationary eigenstates. However, the Floquet theorem tells us that because the Hamiltonian is periodic in time the eigenstates of Eq.(21) can be represented as a superposition of wave functions with energies shifted by $n\hbar\omega$:

$$\Psi_E(x, t) = e^{-iEt/\hbar} \sum_{n=-\infty}^{\infty} \psi_n(x) e^{-in\omega t}. \quad (23)$$

Away from the points $x = -L/2$ and $x = L/2$ the functions $\psi_n(x)$ are a superposition of plane waves

$$\psi_n(x) = a_n e^{ik_n x} + b_n e^{-ik_n x}, \quad (24)$$

where

$$k_n = \sqrt{\frac{2m}{\hbar^2} (E + n\hbar\omega)}$$

with $Re[k_n] \geq 0$ and $Im[k_n] \geq 0$. At $x = -L/2$ and $x = L/2$ we have the boundary conditions

$$\Psi_E(-\frac{L}{2} - 0, t) = \Psi_E(-\frac{L}{2} + 0, t),$$

$$\Psi_E(\frac{L}{2} - 0, t) = \Psi_E(\frac{L}{2} + 0, t),$$

$$\begin{aligned} \frac{\partial \Psi_E(x, t)}{\partial x} \Big|_{x=-\frac{L}{2}+0} - \frac{\partial \Psi_E(x, t)}{\partial x} \Big|_{x=-\frac{L}{2}-0} \\ = \frac{2m}{\hbar^2} V_{01}(t) \Psi_E(-\frac{L}{2}, t), \end{aligned} \quad (25)$$

$$\begin{aligned} \frac{\partial \Psi_E(x, t)}{\partial x} \Big|_{x=\frac{L}{2}+0} - \frac{\partial \Psi_E(x, t)}{\partial x} \Big|_{x=\frac{L}{2}-0} \\ = \frac{2m}{\hbar^2} V_{02}(t) \Psi_E(\frac{L}{2}, t). \end{aligned}$$

In the case under consideration (i.e., when an electron with energy E comes from $x = -\infty$) the functions $\psi_n(x)$ are

$$\psi_n(x < 0) = \delta_{n,0} e^{ik_n x} + R_n e^{-ik_n x},$$

$$\psi_n(0 < x < L) = A_n e^{ik_n x} + B_n e^{-ik_n x}, \quad (26)$$

$$\psi_n(x > L) = T_n e^{ik_n x}.$$

Here the coefficients R_n and T_n for propagating modes (for which $E_n > 0$) are the amplitudes of reflection from or transmission through the double barrier system absorbing ($n > 0$) or emitting ($n < 0$) an energy $|n|\hbar\omega$, respectively.

Substituting Eq.(23) and Eq.(26) into the boundary conditions Eq.(25) we obtain

$$\begin{aligned} R_n &= (A_n - \delta_{n,0}) e^{-ik_n L} + B_n, \\ T_n &= A_n + B_n e^{-ik_n L}, \end{aligned} \quad (27)$$

where the coefficients A_n and B_n are subject to recursive equations. It is convenient to represent these equations in a matrix form

$$\begin{aligned} \hat{U}_n \begin{pmatrix} A_n \\ B_n \end{pmatrix} + \delta_{n,0} \begin{pmatrix} -ik_0 e^{-ik_0 \frac{L}{2}} \\ 0 \end{pmatrix} \\ = \hat{D}_{n+1} \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} + \hat{I}_{n-1} \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix}. \end{aligned} \quad (28)$$

Here we have introduced the matrices

$$\hat{U}_n = \begin{pmatrix} (ik_n - p_{01}) e^{-ik_n \frac{L}{2}} & -p_{01} e^{ik_n \frac{L}{2}} \\ -p_{02} e^{ik_n \frac{L}{2}} & (ik_n - p_{02}) e^{-ik_n \frac{L}{2}} \end{pmatrix}, \quad (29)$$

$$\hat{D}_{n+1} = \begin{pmatrix} p_{11} e^{i\varphi_1} e^{-ik_{n+1} \frac{L}{2}} & p_{11} e^{i\varphi_1} e^{ik_{n+1} \frac{L}{2}} \\ p_{12} e^{i\varphi_2} e^{ik_{n+1} \frac{L}{2}} & p_{12} e^{i\varphi_2} e^{-ik_{n+1} \frac{L}{2}} \end{pmatrix}, \quad (30)$$

$$\hat{I}_{n-1} = \begin{pmatrix} p_{11} e^{-i\varphi_1} e^{-ik_{n-1} \frac{L}{2}} & p_{11} e^{-i\varphi_1} e^{ik_{n-1} \frac{L}{2}} \\ p_{12} e^{-i\varphi_2} e^{ik_{n-1} \frac{L}{2}} & p_{12} e^{-i\varphi_2} e^{-ik_{n-1} \frac{L}{2}} \end{pmatrix}, \quad (31)$$

where the parameters are: $p_{ij} = V_{ij} m / \hbar^2$, $i = 0, 1$, $j = 1, 2$.

To solve the equation (28) we have generalized the method used in Ref. 36 for a single oscillating delta-function potential.

First of all we consider Eq.(28) at $n > 0$. We suppose that there exist matrices \hat{X}_n such that

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \hat{X}_n \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix}. \quad (32)$$

Then substituting the above constraint into Eq.(28) we obtain a simple recursive equation for the matrices \hat{X}_n ($n > 0$)

$$\hat{X}_n = \left(\hat{U}_n - \hat{D}_{n+1} \hat{X}_{n+1} \right)^{-1} \hat{I}_{n-1}. \quad (33)$$

Using these matrices we can express all the coefficients A_n , B_n ($n > 0$) in terms of A_0 and B_0 only

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \hat{X}_n \dots \hat{X}_1 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad n > 0. \quad (34)$$

Further we consider $n < 0$ and introduce the matrices \hat{Y}_n

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \hat{Y}_n \begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix}. \quad (35)$$

The corresponding recursive equation for the matrices \hat{Y}_n is

$$\hat{Y}_n = \left(\hat{U}_n - \hat{I}_{n-1} \hat{Y}_{n-1} \right)^{-1} \hat{D}_{n+1}. \quad (36)$$

Using these matrices we express the coefficients A_n , B_n ($n < 0$) in terms of A_0 and B_0 :

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = \hat{Y}_n \dots \hat{Y}_{-1} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad n < 0. \quad (37)$$

As a final step we consider Eq.(28) at $n = 0$. After simple manipulations we find the coefficients A_0 and B_0 :

$$\begin{aligned} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} &= \left(\hat{U}_0 - \hat{D}_1 \hat{X}_1 - \hat{I}_{-1} \hat{Y}_{-1} \right)^{-1} \\ &\times \begin{pmatrix} ik_0 e^{-ik_0 \frac{L}{2}} \\ 0 \end{pmatrix}. \end{aligned} \quad (38)$$

Thus, using the solutions of the recurrent equations Eq.(33) and Eq.(36) we can calculate all the coefficients A_n , B_n (see Eq.(34), Eq.(37), and Eq.(38)). Note that in each particular case we need to take into account only the limited number $|n| < n_{max}$ of side bands and thus we can put $\hat{X}_{n_{max}+1} \approx 0$ and $\hat{Y}_{-n_{max}-1} \approx 0$.

The coefficients R_n and T_n can be calculated with the help of Eq.(27). For the propagating modes ($E_n \equiv E + n\hbar\omega > 0$) of interest here, these coefficients determine the elements of the Floquet scattering matrix

$$|S_{F,11}(E_n, E)|^2 = \frac{k_n}{k_0} |R_n|^2, \quad (39)$$

$$|S_{F,21}(E_n, E)|^2 = \frac{k_n}{k_0} |T_n|^2.$$

Here the indexes 1 and 2 correspond to the left and right reservoirs, respectively. To obtain the matrix elements $S_{F,22}$ and $S_{F,12}$ we need to solve the same problem with plane waves coming from the right.

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