Optimal Quantum Pumps

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We study adiabatic quantum pumps on time scales that are short relative to the cycle of the pump. In this regime the pump is characterized by the matrix of *energy shift* which we introduce as the dual to Wigner's time delay. The energy shift determines the charge transport, the dissipation, the noise, and the entropy production. We prove a general lower bound on dissipation in a quantum channel and define optimal pumps as those that saturate the bound. We give a geometric characterization of optimal pumps and show that they are noiseless and transport integral charge in a cycle. Finally we discuss an example of an optimal pump related to the Hall effect.

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Introduction.—A time-dependent scatterer can transport charges between electron reservoirs which otherwise are in thermal equilibrium. This makes it into a quantum pump. An example is shown in Fig. 1, where the flux Φ is slowly time dependent. While operating, the pump may also generate (excess) noise in the ideal channels connecting to the reservoirs and dissipate energy in the reservoirs. A pump is adiabatic when its frequency ω is slow compared with the natural time scale τ of the scattered electrons, e.g., the Wigner time delay [1]. The adiabaticity parameter, $\varepsilon = \omega\tau \ll 1$, plays the role analogous to the semiclassical limit: A particle localized in energy is scattered at a well-defined time as measured by the pump cycle.

The theory of adiabatic pumps is concerned with a description of transport and noise in terms of the frozen, on-shell, scattering matrix, $S(t; E)$. In the case when the pump is connected to, say, two reservoirs, as in Fig. 1, S is an $n \times n$ unitary matrix, with n the *total* number of channels in both leads. S is parametrized by the frozen time t and energy E. At low temperatures, $\tau/\beta \ll \hbar$, the transport and noise are determined by the electrons near the Fermi energy, μ, and hence by $S(t; \mu)$.

Two basic results in the theory of adiabatic pumps are [Eq. (3) below] originally due to [2,3], for the *instantaneous* expected current in a channel, and a formula of Levitov and Lesovik [4,5], for the current correlations, and the noise, in a *pump cycle*. Here we focus on further quantities that admit a local description in time, such as dissipation at $\beta = \infty$, which is related to integral transport, and entropy and noise production at $\beta < \infty$.

Energy shift.—It turns out that instantaneous response is determined by the *energy shift* matrix, $\mathcal{E}$. It is conjugate to Wigner time delay, $\mathcal{T}(t, \mu) = -i\hbar\partial_\mu S(t, \mu)S^\dagger(t, \mu)$, and is defined by:

$$\mathcal{E}(t, \mu) = i\hbar\partial_t S(t, \mu)S^\dagger(t, \mu). \tag{1}$$

It is of the order of the adiabaticity parameter ε with matrix elements,

$$\mathcal{E}_{jk} = i\hbar\langle\psi_k\,|\,\dot{\psi}_j\rangle, \tag{2}$$

where $|\psi_j\rangle$ is the jth *row* of the scattering matrix. For example, the diagonal matrix elements of $\mathcal{E}$ determine the instantaneous net current entering the reservoir through the jth channel (even at zero temperature)

$$\dot{Q}_j = \tfrac{e}{h}\,\mathcal{E}_{jj} + O(\varepsilon^2). \tag{3}$$

(A formal derivation of this result follows easily from the analog of Eqs. (10) and (11) below.) As we shall see, the energy shift also provides information on dissipation and noise, and leads to a characterization of optimal pumps.

Lower bound on dissipation.—In order to motivate the notion of an optimal pump we shall first establish a lower bound on the dissipation in a quantum channel.

Suppose a reservoir at zero temperature is connected by a channel to a general *time-independent,* possibly nonthermal, particle source. (In the applications we consider here, this particle source will be an adiabatic quantum pump.) Let $\dot{E}$ denote the net energy flux (power) and $\dot{Q}$ the charge flux (current) flowing out from the source to the cold reservoir. The power dissipated in the channel, i.e., the difference between the energy flow and the energy flow that can be recovered, satisfies the general lower bound,

$$\dot{E} - \frac{\mu}{e}\,\dot{Q} \geq \frac{R_k}{2}\,\dot{Q}^2, \tag{4}$$

with $R_k = h/e^2$ being the (von Klitzing) unit of resistance. This bound does not depend on the nature of the particle source. It is a consequence of the fact that a channel is one dimensional, the charge carriers are noninteracting (spinless) fermions, the reservoir is at zero temperature, and the particle source is time independent. A source that saturates the lower bound [Eq. (4)] will be called optimal.

Proof.—A time-independent particle source connected to a channel is characterized by the filling $0 \leq n(k) \leq 1$ of states at momentum k. Let $\dot{E}$ ($\dot{Q}$) be the energy (charge)

current out of the source and let $\epsilon(k)$ be the dispersion relation. Then,

$$\dot{Q} = \frac{e}{2\pi\hbar}\int_{\epsilon'(k)>0} dk\, n(k)\epsilon'(k),$$
$$\dot{E} = \frac{1}{2\pi\hbar}\int_{\epsilon'(k)>0} dk\, n(k)\epsilon(k)\epsilon'(k). \quad (5)$$

The bathtub principle (with respect to the measure $\epsilon'(k)dk$ on $\{k \mid \epsilon'(k) > 0\}$; see, e.g., [6]) states that for fixed $\dot{Q}$ the quantity $\dot{E}$ is minimized by $n(k) = \theta[\mu - \epsilon(k)]$ for some μ. Assuming $k\epsilon'(k) \geq 0$, $\epsilon(0) = 0$, we find for the minimizer

$$\dot{Q} = \frac{e\mu}{2\pi\hbar}, \qquad \dot{E} = \frac{\mu^2}{4\pi\hbar}. \quad (6)$$

This implies that $\dot{E} \geq \frac{R_k}{2}\dot{Q}^2$, with equality holding if, and only if, the source is a reservoir at thermal equilibrium at zero temperature so that the carriers fill the Fermi sea up to energies μ.

Consider next a channel connecting a particle source, denoted by subscript $(+)$, to a thermal reservoir, denoted by subscript $(-)$, at zero temperature and with chemical potential μ_-. $\dot{E} = \dot{E}_+ - \dot{E}_-$ ($\dot{Q} = \dot{Q}_+ - \dot{Q}_-$) is the net energy (charge) flowing into the cold reservoir. Since the reservoir is at zero temperature, $\dot{E}_- = \frac{R_k}{2}\dot{Q}_-^2 = \frac{\mu_-^2}{2h}$. Meanwhile, $\dot{E}_+$ is at least $\frac{R_k}{2}\dot{Q}_+^2$. Hence $\dot{E} \geq \frac{R_k}{2}(\dot{Q}_+^2 - \dot{Q}_-^2) = \frac{R_k}{2}\dot{Q}^2 + \frac{\mu_-}{e}\dot{Q}$. Equality occurs if, and only if, the source also fills a Fermi sea up to some energy μ_+. Equation (4) bounds the dissipation in an ideal channel.

Optimal pumps.—An adiabatic pump approximates a time-independent (and typically nonthermal) particle source that connects to the n channels. The lower bound [Eq. (4)] motivates the following definition: We say that an adiabatic pump is optimal if the bound [Eq. (4)] is saturated for all times and all channels in the adiabatic limit. Since the left-hand side of Eq. (4) is made of two terms that are each of order ε while the right-hand side is a term of order ε^2, saturating the bound means that equality of the two sides holds to order ε^2.

For the jth channel of an adiabatic pump connected to reservoirs at zero temperature we will establish:

$$\dot{E}_j - \frac{\mu}{e}\dot{Q}_j = \frac{1}{2h}\sum_k |\mathcal{E}_{jk}|^2 + O(\varepsilon^3). \quad (7)$$

It follows from Eqs. (3) and (4) that the jth channel is optimal if $\mathcal{E}_{jk} = 0$ for all $k \neq j$. This leads to a simple criterion for optimal pumps: A pump is optimal if, and only if, the energy shift $\mathcal{E}$ is a diagonal matrix for all times.

The notion of optimal pumps is geometric. This is seen from the fact that the vanishing condition on matrix elements of the energy shift, Eq. (2), is invariant under reparametrization of time.

The space of Hermitian $n \times n$ matrices $\mathcal{E}$ has n^2 real dimensions, while the space of diagonal matrices is n dimensional. In particular, pumps with a single lead and as single channel are automatically optimal. Below we shall give an example of an optimal pump with $n = 2$ that models the quantum Hall effect.

The scattering matrix associated with a diagonal energy shift is $S(t) = U_d(t)S_0$, where $U_d(t)$ is a *diagonal* unitary and S_0 is a constant unitary matrix. According to [7], this special form of an S matrix turns out to characterize noiseless pumps in the theory of Levitov and Lesovik. Optimal pumps are therefore distinguished in more than one way. In [5] weak pumping at zero temperature is studied. This leads to a different characterization of optimal pumps.

Integral charge transport.—Optimal channels transport integral charge in a cycle of the pump. This can be seen from Eq. (3) for the jth channel,

$$\frac{Q_j}{e} = -\frac{i}{2\pi}\int \langle\psi_j \mid \dot{\psi}_j\rangle\, dt = -\frac{i}{2\pi}\oint \langle\psi_j \mid d\psi_j\rangle. \quad (8)$$

For an optimal channel, $|\dot{\psi}_j\rangle$ is parallel to $|\psi_j\rangle$, since $\langle\psi_k \mid \dot{\psi}_j\rangle = 0$; hence it can only accumulate a phase along the path. Since $|\psi_j\rangle$ is single valued, the total phase accumulated on a closed path must be an integer multiple of 2π. It is worth remarking that in this case Eq. (8) not only expresses the expectation value of the charge transport in a cycle, as it does by virtue of its derivation, but also the actual charge transport, since the stated condition implies absence of noise, i.e., vanishing variance.

The right-hand side of Eq. (8) shows that charge transport is geometric: It depends on the path but is independent of its parametrization. In spite of this geometric interpretation, the charge transport is *not quantized* in the sense that it has no topological content: A small deformation of the scattering matrix will be a deformation away from optimality and will deform the charge transport away from the integers.

Geometric interpretation.—The dissipation formulas admit a geometric interpretation. $|\psi_j\rangle$, being normalized, can be viewed as a point on the sphere $S^{2n-1} \subset \mathbb{C}^n$. The Hopf map [8] $\pi : S^{2n-1} \to \mathbb{C}P^{n-1}$, which "forgets" the phase of $|\psi\rangle$, turns S^{2n-1} into a fiber (circle) bundle with base space $\mathbb{C}P^{n-1}$. The jth row of $\mathcal{E}$ describes the velocity of $|\psi_j\rangle$ in S^{2n-1}. Of this, $\mathcal{E}_{jj}$ is the projection of this velocity onto the fiber—the changing phase of $|\psi_j\rangle$—while the matrix elements $\mathcal{E}_{jk}$, with $k \neq j$, give the projection of this velocity onto $\mathbb{C}P^{n-1}$. The current $\dot{Q}_j$, and the minimal dissipation $|\mathcal{E}_{jj}|^2/4\pi$ are both functions of motion in the fiber, while the excess dissipation is the "energy" (that is, squared velocity) associated with motion in the base.

Entropy and noise.—So far we have not considered correlations between the current (or power) at different times. Entropy and noise production involve such correlations. The analysis depends critically on which of the two small parameters, $\hbar\omega$ and β^{-1}, is smaller.

If $\hbar\omega \ll \beta^{-1} \ll \hbar/\tau$ (e.g., in the experiment of Switkes *et al.* [9]), then the correlations between current (and power) at different portions of a cycle are negligible, and one can meaningfully speak of the entropy (noise) production per unit time $\dot{S}_j$ ($\dot{N}_j$) in the jth channel. We remark, without proof, that these quantities, too, are determined by the energy shift and are proportional to the *excess* energy dissipation:

$$\dot{S}_j = \frac{\beta}{4\pi\hbar}\sum_{k\neq j}|\mathcal{E}_{jk}|^2, \qquad \dot{N}_j = \frac{\beta e^2}{12\pi\hbar}\sum_{k\neq j}|\mathcal{E}_{jk}|^2. \quad (9)$$

If $\beta^{-1} \ll \hbar\omega$, however, then the analysis is fundamentally nonlocal in time, and one is naturally led to study the noise or entropy generated by a complete cycle. The results then have a different character [4,5].

Dissipation in adiabatic pumps.—To derive Eq. (7), we note that the left-hand side of Eq. (7) can be written as

$$\dot{E}_j - \frac{\mu}{e}\dot{Q}_j = \int \frac{dE}{2\pi\hbar}(E-\mu)[n_{+j}(E) - n_-(E)]. \quad (10)$$

where $n_-(E) = \theta(\mu - E)$ is the distribution of the electrons that arrive from the (zero temperature) reservoirs and $n_{+j}(E)$ is the distribution of the electrons that enter the jth reservoir. The pump scrambles the incoming distribution and produces a (nonthermal) outgoing distribution $n_{+j}(E)$. Calculating the outgoing distribution is a problem in adiabatic scattering theory.

We will show that the outgoing density at energy E, on the jth channel, is

$$[n_+(E)]_{jj} \approx \theta(\mu - E) + [\mathcal{E}_{jj} + O(\varepsilon^2)]\delta(E-\mu) - (\mathcal{E}^2)_{jj}\delta'(E-\mu)/2, \quad (11)$$

where ($\approx$) means that the operator on the left-hand side can be approximated by the semiclassical distributions (symbol) on the right-hand side to second order in ε. Inserting this into Eq. (10), and using the fact that $(\mathcal{E}^2)_{jj} = \sum_{k=1}^{n}|\mathcal{E}_{jk}|^2$, gives Eq. (7). This relation establishes an instantaneous identity between charge and energy transports (which are first order) and dissipation (which is second order). This is remarkable because S gives only the leading adiabatic approximation to the scattering matrix and is therefore inadequate to describe general second order processes and first order processes beyond the leading behavior. In particular, neither $\dot{E}$ nor $\dot{Q}$ are correctly computable to second order in ε but Eq. (7) is. Equation (3) is derived along similar, though somewhat simpler, lines.

Adiabatic scattering.—It remains to derive Eq. (11). We start with the standard point of view [10] of time-dependent scattering theory, which views the S matrix as a comparison of a "free" dynamics, generated by H_0, and the interacting dynamics, generated by $H(t)$. For example, we can pick for H_0 the Hamiltonian associated with disconnected channels. Let $U(t,s)$ and $U_0(t,s)$ denote the corresponding evolutions. Then, the S matrix is defined by the limit (which we assume exists)

$$S_d(t) = \lim_{T\to\infty} U_0(t,T)U(T,-T)U_0(-T,t). \quad (12)$$

In the absence of a scatterer, $U = U_0$ and S is the identity, as it should be. When the scatterer is time independent, $H(t) = H$, the existence of the $T \to \infty$ limit for the factors $U(0,-T)U_0(-T,t)$ and $U_0(t,T)U(T,0)$ implies that $S_d(t)$ is independent of t, as it should be.

$S_d(t)$ maps the incoming wave packet to outgoing ones. When applied to a wave packet near the scatterer, it describes the mapping for an incoming wave, originating at the reservoirs, that hits the scatterer at time t.

It follows from Eq. (12) that, provided the limit exists,

$$i\hbar\dot{S}_d(t) = [H_0, S_d(t)]. \quad (13)$$

This shows that the free dynamics controls when a wave packet hits the scatterer. Equation (13) determines $n_+(H_0)$ to be

$$S_d(t)n_-(H_0)S_d(t)^\dagger = n_-[H_0 - i\hbar\dot{S}_d(t)S_d(t)^\dagger]. \quad (14)$$

In the time-independent case, $\dot{S}_d = 0$, and Eq. (14) is an expression of conservation of energy. For time-dependent scattering, Eq. (14) describes the scattering out of the energy shell. This is the motivation for calling $i\hbar\dot{S}_d(t)S_d(t)^\dagger$ the operator of energy shift.

In the adiabatic limit, the (exact) time-dependent scattering matrix $S_d(t)$ can be approximated by the time-independent scattering matrix for the scatterer frozen at the time of the scattering t. Namely, $S_d(t) \approx \delta(\mu - \mu')S(t;\mu)$, with $S(t;\mu)$ being the on-shell scattering matrix of Eq. (1). For the on-shell densities, Eq. (14) takes the form

$$n_+(E,t) = n_-[E - i\hbar\dot{S}_d(t)S_d(t)^\dagger + O(\varepsilon^2)]. \quad (15)$$

A semiclassical expansion of the operator on the right-hand side, restricted to the jth channel, gives Eq. (11).

An optimal pump.—An example of an optimal pump is shown schematically in Fig. 1. Each of the two leads, each leading having one channel, is connected to a reservoir at zero temperature on one end and to the loop of circumference ℓ on the other end. The loop is threaded by a time-dependent magnetic flux Φ, which is the engine of the pump. The scattering at the vertices is a permutation matrix corresponding to the arrows in the figure. The frozen

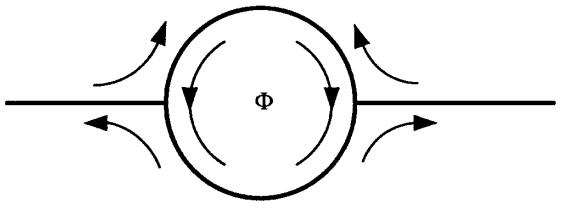

FIG. 1. An optimal quantum pump represented by a graph of ideal wires. For a fixed value of the magnetic flux, Φ, particles that enter from the left go clockwise around the loop and exit to the left, while particles that enter from the right go counterclockwise and exit to the right.

scattering matrix of the pump is therefore diagonal, with the phases of the two reflection coefficients determined by Φ:

$$r = e^{i(k\ell+\Phi)}, \qquad r' = e^{i(k\ell-\Phi)}. \tag{16}$$

From Eq. (8), we see that increasing Φ by a unit of quantum flux draws one particle in from the right and expels one particle to the left. This is independent of the chemical potential μ of the bath, the circumference ℓ of the loop, and the position of the vertices on the loop.

At first glance the pumping expressed by Eq. (8) seems to be in conflict with common sense: The frozen S matrix does not allow transmission across the scatterer, so how can the pump transport any charge at all? This can be understood as follows. Increasing the flux creates an EMF around the loop that accelerates the clockwise-moving particles and decelerates the counterclockwise-moving particles. In particular, some of the low-energy counterclockwise movers that entered from the right are turned around by the EMF and become clockwise movers, after which they emerge to the left. This accounts for the net transfer of charge from right to left. Since the scattering at each vertex is deterministic, the outgoing channels have no entropy, the inequalities (4) become equalities, and the pump is optimal. A little reflection shows that Fig. 1 is a graph theoretic description of the quantum Hall effect. In the quantum Hall effect, time reversal is broken by an external magnetic field. In Fig. 1, time reversal is broken by the permutation matrix associated with the scattering condition at the vertices. More precisely, the vertex conditions at the vertices can be implemented by the edge currents in the quantum Hall effect in a Corbino disk [11].

Concluding remarks.—We have analyzed quantum pumps as a problem in adiabatic scattering theory. We have focused on transport properties that admit instantaneous description, i.e., on times scales that are small compared to the pump cycle. In this theory a central role is played by the matrix of energy shift. We proved a general bound on the dissipation in quantum channels that motivated a notion of optimal quantum pumps. Optimal quantum pumps have geometric significance [12], saturate a bound on dissipation; transport integer charges in closed cycles, are noiseless, and minimize entropy production. Finally, we showed that the integer quantum Hall effect may be interpreted as an optimal pump.

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Note added.—Shortly after submission of this Letter, Makhlin and Mirlin [12] derived interesting geometric results for noise in pumps. Some of their results overlap with some of ours.

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