Optimal Quantum Pumps

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Optimal pumps saturate a lower bound on energy dissipation. We give a characterization of optimal pumps in terms of the *energy shift* matrix, which is computed from the on-shell, frozen, scattering matrix. The energy shift determines the charge transport, the dissipation and entropy production in adiabatic pumps. We give a geometric characterization of optimal pumps and discuss an example.

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Overview: Quantum pumps transport charge, spin, energy, entropy, etc. in and out of electron reservoirs which are themselves at equilibrium and at identical chemical potentials, μ, and identical temperatures, $1/\beta$. The pumping is done by scattering from a time dependent scatterer [1–8].

Let $\dot{E}$ denote the net energy flux (power) and $\dot{Q}$ the charge flux (current) in a given channel, flowing out from the scatterer to a distant reservoir. Let $R_k = h/e^2 \approx 25812.80\,\Omega$ be the (von Klitzing) quantum unit of resistance. If the reservoir is held at zero temperature, we shall prove an elementary lower bound on the power dissipated at each and every channel:

$$\dot{E} - \frac{\mu}{e}\dot{Q} \geq \frac{R_k}{2}\,\dot{Q}^2. \tag{1}$$

If $R_k/2$ is interpreted as the contact resistance of each channel, the right hand side gives the dissipation at the contact. This bound does not depend on the adiabaticity of the pump. It is a consequence of the fact that a channel is one dimensional, that the charge carriers are non-interacting fermions and the reservoirs are at zero temperature. Channels that saturate the lower bounds Eq. (1) will be called optimal. An pump is called optimal if all of its channels are optimal.

We henceforth use units with $e = \hbar = 1$, so $R_k = 2\pi$ and the chemical potential can be interpreted as a voltage.

Adiabatic pumps admit an explicit characterization of optimal channels in terms of their scattering matrix. A pump is adiabatic when the frequency ω of the pump is slow compared with the natural time scale τ of the problem, [9], e.g., the Wigner time delay [10]. That is, $\varepsilon = \omega\tau \ll 1$.

Let $\mathcal{S}(t;\mu)$ be the (time independent) scattering matrix at energy μ, for a scatterer frozen at time t. In the case of n channels, $\mathcal{S}(t;\mu)$ is an $n \times n$ unitary matrix. $\dot{\mathcal{S}}(t;\mu) = O(\varepsilon)$ denotes the t derivative of the matrix. The *energy shift* matrix, $\mathcal{E}$, is defined to be:

$$\mathcal{E}(t,\mu) = i\hbar\,\dot{\mathcal{S}}(t,\mu)\mathcal{S}^\dagger(t,\mu), \tag{2}$$

and is of order ε. The matrix elements of the energy shift can be expressed as:

$$\mathcal{E}_{jk} = i\hbar\,\langle\psi_k|\dot{\psi}_j\rangle \tag{3}$$

where $|\psi_j\rangle$ is the j-th row (not column!) of the scattering matrix. The energy shift is conjugate to the Wigner time delay $\mathcal{T}(t,\mu) = -i\hbar\,\partial_\mu\mathcal{S}(t,\mu)\mathcal{S}^\dagger(t,\mu)$, [10].

The energy shift plays a role in adiabatic pumping. For example, it is known that the diagonal matrix elements of $\mathcal{E}$ determine the net current entering the reservoir through the j-th channel [1,3,6]

$$\dot{Q}_j = \mathcal{E}_{jj}/2\pi + O(\varepsilon^2). \tag{4}$$

As we shall see, the energy-shift also provides information on dissipation and noise.

For a channel connected to a reservoir at zero temperature we shall show:

$$\dot{E}_j - \mu\dot{Q}_j = \frac{1}{4\pi}\sum_k |\mathcal{E}_{jk}|^2 + O(\varepsilon^3). \tag{5}$$

It follows that the j-th channel is optimal if $\mathcal{E}_{jk} = 0$ for $j \neq k$, and the pump is optimal if and only if $\mathcal{E}$ is a diagonal matrix.

The scattering matrix of an optimal pump is $\mathcal{S}(t) = U_d(t)\mathcal{S}_0$ where $U_d(t)$ is a *diagonal* unitary and $\mathcal{S}_0$ a constant unitary matrix. This coincides with Andreev and Kamenev's characterization of noiseless pumps [11,16].

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. (3) is invariant under reparameterization of time.

For n-channel scattering, the space of Hermitian matrices $\mathcal{E}$ has n^2 real dimensions, while the space of diagonal matrices is n dimensional. Optimal pumps are therefore a set of codimension $n^2 - n$. In particular, pumps with a single channel are automatically optimal. Below we shall give an example of an optimal pump with $n = 2$ that models the quantum Hall effect.

Optimal channels are related to integral charge transport: If the j-th channel is optimal, then the charge transport in a cycle of the pump is an integer. This can be seen from Eq. (4):

$$Q_j = -\frac{i}{2\pi}\int\langle\psi_j|\dot{\psi}_j\rangle\, dt = -\frac{i}{2\pi}\oint\langle\psi_j|d\psi_j\rangle. \qquad (6)$$

For an optimal channel $|\dot{\psi}_j\rangle$ is parallel to $|\psi_j\rangle$, since $\langle\psi_k|\dot{\psi}_j\rangle = 0$, 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. (6) 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., variance. The right hand side of Eq. (6) shows that charge transport is geometric: It depends on the path but is independent of its parameterization. In spite of all of this, the charge transport is not quantized and 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. In [4,5] it is argued that non-dissipative processes make quantum pumps similar to systems with energy gaps where charge transport is related to topological invariants. Although the conclusion about integrality of transport is correct for optimal pumps, the argument is misleading because the charge transport in pumps is not associated with topological invariants. Moreover, it is not possible on the basis of the order of dissipation alone to distinguish between optimal and non-optimal channels; in either case the dissipation is $O(\varepsilon^2)$. It is however true that absence of *excess* dissipation implies integrality.

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 [13] $\pi: S^{2n-1}\to\mathbb{C}P^{n-1}$, 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 j-th 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.

Finally, we remark, without proof [14], that the entropy flow into a cold reservoir, $\beta\gg\hbar/\tau$, from a slowly operated pump, $\hbar\omega\ll\beta^{-1}$ [15], is proportional to the excess energy dissipation, and not to the total energy dissipation:

$$\dot{S}_j = \frac{\beta}{4\pi}\sum_{k\neq j}|\mathcal{E}_{jk}|^2. \qquad (7)$$

A lower bound on dissipation: We first consider a single channel and let $\dot{E}_\pm$ ($\dot{Q}_\pm$) be the energy (charge) current transported across it by the outgoing (+) or incoming (−) carriers separately. Then

$$\dot{E}_\pm \geq \pi\dot{Q}_\pm^2, \qquad (8)$$

with equality holding if and only if the carriers fill a Fermi sea up to chemical potentials $\mu_\pm$. Here is why. Let $0\leq n(k)\leq 1$ be the filling of states at momentum k and energy $\epsilon(k)$, which move with velocity $\epsilon'(k)$. Then

$$\begin{aligned}\dot{Q}_+ &= \frac{1}{2\pi}\int_{\epsilon'(k)>0} dk\, n(k)\epsilon'(k),\\ \dot{E}_+ &= \frac{1}{2\pi}\int_{\epsilon'(k)>0} dk\, n(k)\epsilon(k)\epsilon'(k).\end{aligned} \qquad (9)$$

The bathtub principle (w.r.t. the measure $\epsilon'(k)dk$ on $\{k\mid\epsilon'(k)>0,\}$; see e.g., [16]) 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

$$\dot{Q}_+ = \frac{\mu_+}{2\pi}, \qquad \dot{E}_+ = \frac{\mu_+^2}{4\pi}, \qquad (10)$$

which proves (8).

Consider next a channel connected to a reservoir at chemical potential μ_-. Let $\dot{E}=\dot{E}_+-\dot{E}_-$ ($\dot{Q}=\dot{Q}_+-\dot{Q}_-$) be the net energy (charge) flowing into the reservoir (i.e., out of the system). Then $\dot{E}_-=\pi\dot{Q}_-^2=\mu_-^2/4\pi$, while $\dot{E}_+$ is at least $\pi\dot{Q}_+^2$. We compute

$$\dot{E}\geq\pi(\dot{Q}_+^2-\dot{Q}_-^2)=\pi\dot{Q}^2+\mu_-\dot{Q}. \qquad (11)$$

This is Eq. (1) in natural units, and equality occurs if and only if the flow into the reservoir also fills a Fermi sea with Fermi energy μ_+. Note that (1) gives the dissipation in each lead [17].

Dissipation in adiabatic pumps: To derive Eq. (5), we note that the left hand side of Eq. (5) can be written as

$$\dot{E}_j-\mu\dot{Q}_j=\frac{1}{2\pi}\int dE(E-\mu)\big(n_{+j}(E)-n_-(E)\big). \qquad (12)$$

where $n_-(E)=\theta(E-\mu)$ 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 reservoirs. The pump scrambles the incoming distribution and produces a (non-thermal) outgoing distribution $n_{+j}(E)$. To calculate the outgoing distribution is a problem in adiabatic scattering theory.

Our basic tool is a formula which relates outgoing and incoming distribution in the adiabatic limit. Let $|e_k\rangle$ denote the eigenvectors of $\mathcal{E}$ with eigenvalue e_k. The outgoing density at energy E, on the j-th channel, is

$$n_{+j}(E) \approx \sum_k n_-(E-e_k)|\langle e_k|j\rangle|^2, \tag{13}$$

where $\approx$ means that this is an equality for distributions, to leading order in ε. Inserting this in Eq. (12) we obtain

$$\dot{E}_j - \mu\dot{Q}_j = \frac{1}{4\pi}\sum_{k=1}^n e_k^2|\langle e_k|j\rangle|^2 = \frac{1}{4\pi}\sum_{k=1}^n |\mathcal{E}_{jk}|^2. \tag{14}$$

Adiabatic scattering: It remains to derive Eq. (13). We start with the standard point of view [18] 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)

$$\mathcal{S}_d(t) = \lim_{T\to\infty} U_0(t,T)U(T,-T)U_0(-T,t). \tag{15}$$

In the absence of a scatterer, $U=U_0$ and $\mathcal{S}$ 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 $\mathcal{S}_d(t)$ is independent of t, as it should.

$\mathcal{S}_d(t)$ maps 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. (15) that, provided the limit exists,

$$i\,\dot{\mathcal{S}}_d(t) = [H_0, \mathcal{S}_d(t)]. \tag{16}$$

The free dynamics controls when a wave packet hits the scatterer. Eq. (16) determines $n_+(H_0)$ to be

$$\mathcal{S}_d(t)n_-(H_0)\mathcal{S}_d(t)^\dagger = n_-\big(H_0 - i\dot{\mathcal{S}}_d(t)\mathcal{S}_d(t)^\dagger\big). \tag{17}$$

In the time independent case, $\dot{\mathcal{S}}_d = 0$, and Eq. (17) is an expression of conservation of energy. For time dependent scattering, Eq. (17), describes the scattering out of the energy shell. This is the motivation for calling $i\dot{\mathcal{S}}_d(t)\mathcal{S}_d(t)^\dagger$ the operator of energy shift.

In the adiabatic limit, the (exact) time dependent scattering matrix $\mathcal{S}_d(t)$ can be approximated by the time independent scattering matrix for the scatterer frozen at the time of the scattering t. Namely, $\mathcal{S}_d(t) \approx \delta(\mu-\mu')\,\mathcal{S}(t;\mu)$, with $\mathcal{S}(t;\mu)$ the on-shell scattering matrix of Eq. (2). For the on-shell densities Eq. (17) takes the form

$$n_+(\mu,t) \approx n_-\big(\mu - \mathcal{E}\big), \tag{18}$$

which is a matrix version of Eq. (13).

A 2-lead optimal pump: We conclude with an example of a nontrivial optimal pump. Besides demonstrating the possibility of optimal pumps with multiple leads, this example serves as a schematic of the quantum Hall effect.

The pump, shown in Fig. (1), has two channels, each connected to a reservoir on one end and to a loop of circumference ℓ on the other. The loop is threaded by 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. 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. The scattering matrix of the pump is therefore diagonal, with the phases of the two reflection coefficients determined by Φ:

$$r = e^{i(k\ell+\Phi)}, \quad r' = e^{i(k\ell-\Phi)}. \tag{19}$$

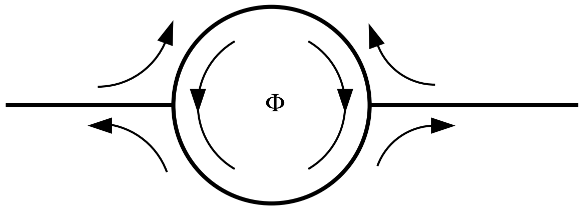

FIG. 1. A graph associated with the quantum Hall effect.

From Eq. (6), 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, and independent of the circumference ℓ of the loop.

At first glance this seems impossible, since there is no transmission across the scatterer. However, there is a simple semiclassical explanation. Increasing the flux creates an EMF around the loop that accelerates the clockwise-moving particles and decelerates the counterclockwise-moving particles. Thus the outgoing states on the left lead are filled to a higher energy than the outgoing states on the right. Furthermore, some low-energy counterclockwise-movers that entered from the right are actually 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 (9) become equalities, and the pump is optimal.

The quantum Hall effect can be described by a scatterer with four leads (north, south, east and west) with a north-south voltage and an east-west current. However, if the the north and south leads are connected by a wire, and if the resulting loop is threaded by a time-varying magnetic flux to generate the north-south voltage, then one obtains a geometry shown in Fig. (2).

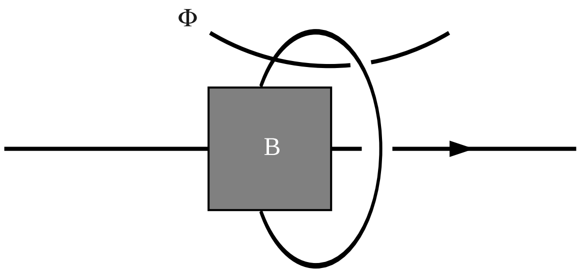

FIG. 2. The Hall effect as a pump driven by the emf $\dot{\Phi}$.

Indeed, the pump of Figure 1 models the essential features of the integer QHE, [22]. The Hall crystal, and the magnetic field applied to the Hall crystal, are modeled by the vertices, which scatter particles in a time-asymmetric manner. The "clockwise movers" of Figure 1 correspond to electrons that enter the Hall crystal from the west, move along the edge of the crystal until they reach the south lead, go along the loop from south to north, move along the edge from north to west, and emerge to the west. The "counterclockwise movers" correspond to electrons that go from east to north (along the Hall crystal) to south (along the loop) and then to east and out the east lead. By standard arguments [19], the edge states reflect the existence of localized bulk states in the crystal.

Concluding remarks: Adiabatic theory divides into two chapters: One deals with systems with *discrete spectra* and the other with systems with *continuous spectra*. This division carries over to the theory of adiabatic transport. For systems with discrete spectra interesting transport properties often require that the system is multiply connected, see e.g., [20]; charge transport admits a geometric interpretation, and is related to Chern numbers. Here we have analyzed quantum pumps as a problem in adiabatic scattering theory. It is known that charge transport in a closed cycle of a pump is, again, geometric [3,6]. But, unlike the discrete situation, charge transport is not quantized in the sense that it is not related to interesting topological invariants. Here we introduced the notion of optimal quantum pumps, which is again a geometric notion. Optimal pumps saturate a bound on dissipation, transport integer charges in closed cycles, are noiseless and minimize entropy production. We gave an explicit characterization of optimal pumps in terms of the matrix of *energy shift*.

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