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Transport and Dissipation in Quantum Pumps

J. E. Avron,[1] A. Elgart,[2] G. M. Graf,[3] and L. Sadun[4]

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This paper is about adiabatic transport in quantum pumps. The notion of "energy shift," a self-adjoint operator dual to the Wigner time delay, plays a role in our approach: It determines the current, the dissipation, the noise and the entropy currents in quantum pumps. We discuss the geometric and topological content of adiabatic transport and show that the mechanism of Thouless and Niu for quantized transport via Chern numbers cannot be realized in quantum pumps where Chern numbers necessarily vanish.

KEY WORDS: Quantum pumps; energy shift; current; dissipation; entropy; noise; Berry phase; Weyl calculus.

To Elliott Lieb, a mentor and friend, on the occasion of his 70 th birthday.

1. INTRODUCTION

An adiabatic quantum pump[11, 13, 16] is a time-dependent scatterer connected to several leads. Figure 1 is an example with two leads. Each lead may have several channels. The total number of channels, in all leads, will be denoted by n. Each channel is represented by a semi-infinite, one dimensional, (single mode) ideal wire. We assume that the particles propagating in the channels are non-interacting[5] and all have dispersion $\epsilon(k)$. For the sake of concreteness we shall take quadratic dispersion, $\epsilon(k) = k^2/2$, but most of our results carry over to more general dispersions. We also assume that the incoming particles are described by a density matrix

[1] Department of Physics, Technion, 32000 Haifa, Israel; e-mail: avron@physics.technion.ac.il
[2] Courant Institute of Mathematical Sciences, New York, New York 10012.
[3] Theoretische Physik, ETH-Hönggerberg, 8093 Zürich, Switzerland.
[4] Department of Mathematics, University of Texas, Austin, Texas 78712.
[5] Quantum pumps have also been discussed in the context of interacting electrons, see, e.g., refs. 2 and 33.

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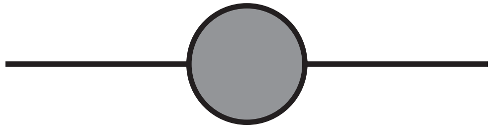

Fig. 1. A model of a quantum scatterer with two leads.

ρ common to all channels: $\rho(E) = (1 + e^{\beta(E-\mu)})^{-1}$, with chemical potential μ and temperature T. The scatterer is adiabatic when its characteristic frequency $\omega \ll 1/\tau$, with τ the typical dwell time in the scatterer. We take units so that $k_B = \hbar = m = e = +1$.

The central questions about an adiabatic quantum pump concern how particles are transported from one lead to another by the pump. What is the expected charge transport per unit time (or per cycle)? How much energy is dissipated in the process? How much statistical fluctuation (noise and entropy) is expected in the current? How are energy dissipation and entropy production related? How can these quantities be minimized?

The first of these questions was addressed by Büttiker, Prêtre, and Thomas[(16)] (BPT) in the context of linear response theory. They derived a formula for the expected current as a function of the scattering matrix and its time derivative. (Some of the elements of their derivation can be found, though in a rather different form, in Section 4.2.) Subsequent work, both theoretical and experimental, explored the significance of the BPT formula. Interest in the subject was piqued by Brouwer's rewriting the BPT formula as an area integral,[(11)] and by the experiments of ref. 36. (It is unclear whether the latter actually represents an adiabatic quantum pump, as alternative explanations[(12)] have been proposed.)

In this paper we address all of the above questions, and see that the answers all depend on a single quantity: the *matrix of energy shift*, constructed below from the scattering matrix and its first derivative in time. The expected transport, described by the BPT formula, is given by the diagonal elements of the matrix of energy shift and appear at order ω^1. Expected energy dissipation, noise, and entropy production depend on the off-diagonal matrix elements, and appear at order ω^2. One might hope that these expressions are the leading terms of an asymptotic expansion in powers of ω, with coefficients computable from the scattering matrix and its derivatives, but no such expansion exists. We construct examples with identical scattering matrices, but whose charge and energy transports agree only to leading order.

An incoming particle sees a quasi-static scatterer.[(15)] The scattering can therefore be computed, to leading order, by time-independent quantum mechanics, using the scattering Hamiltonian in effect at the time that the particle reaches the scatterer. In other words, we pretend that the Hamiltonian always was, and always will be, the Hamiltonian seen by the particle at the time of passage. This gives the "frozen S-matrix." Since time-independent systems conserve energy, so does the frozen S-matrix. We denote by $S(E, t)$ the on-shell frozen S-matrix.

The frozen S-matrix $S(E, t)$ can be viewed in two ways. On the one hand, it is the matrix that gives the amplitudes of outgoing plane waves in the n channels in terms of the amplitudes of incoming plane waves. In abstract scattering theory, however, the S-matrix is an operator that compares time evolution via the actual Hamiltonian $H(t)$ to time evolution via a reference Hamiltonian H_0. If $H(t)$ is independent of time, then the (abstract) S-matrix conserves energy; if H_0 is chosen correctly, then the energy-E fiber of this operator is the same matrix $S(E, t)$.

The outgoing states have, to order ω^0, the same occupation density as the incoming states (since $S(E, t)$ is unitary, and the incoming densities are the same for all channels). This implies no net transport. However, at order ω, there is an interesting interference effect: An incoming particle of well-defined energy does not have a well-defined time of passage. This spread in time is a consequence of the uncertainty principle, and is not related to the dwell time of the particle in the scatterer. Thus, even if $\omega \ll 1/\tau$, the (frozen) S-matrix seen by the tail of the wave packet will differ slightly from that seen by the head of the wave packet. This differential scattering causes the outgoing occupation densities to differ from the incoming densities to order ω^1, leading to a nonzero transport.

The density matrix for the outgoing states, ρ_{out}, is determined by the density matrix $\rho(H_0)$ of the incoming states, and by the S-matrix. Let S_d be the exact (dynamical) S-matrix, computed from the time-dependent Hamiltonian $H(t)$. As we shall explain in Section 4, ρ_{out} is given by

$$\rho_{\text{out}} = \rho(H_0 - \mathscr{E}_d), \qquad \mathscr{E}_d = i\dot{S}_d S_d^*. \tag{1.1}$$

A dot denotes derivative with respect to time.[6] $\mathscr{E}_d$ is the operator of energy shift introduced in ref. 27. It combines information on the state of the scatterer with its rate of change $\dot{S}_d$. For time independent scattering, $\mathscr{E}_d = 0$ and Eq. (1.1) is an expression of conservation of energy. The formula for ρ_{out}, Eq. (1.1), holds independently of whether the scattering is adiabatic or not.

We call the frozen analog of the operator $\mathscr{E}_d$ the *matrix* of energy shift. It is the $n \times n$ matrix

$$\mathscr{E}(E, t) = i\dot{S}(E, t)\, S^*(E, t), \tag{1.2}$$

[6] The time dependence of S_d is discussed in Section 4.

and is a natural dual to the more familiar Wigner time delay[18]

$$\mathcal{T}(E, t) = -iS'(E, t)\, S^*(E, t), \tag{1.3}$$

where prime denotes derivative with respect to E. As we shall see in Section 6.3 their commutator

$$\Omega = i[\mathcal{T}, \mathcal{E}] \tag{1.4}$$

has a geometric interpretation of a curvature in the time-energy plane, analogous to the adiabatic curvature.

Adiabatic transport can be expressed in terms of the matrix of energy shift. For example, the BPT[16] formula for the expectation value of the current in the jth channel, $\langle \dot{Q} \rangle_j$ takes the form:

$$\langle \dot{Q} \rangle_j\, (t) = -\frac{1}{2\pi} \int_0^\infty dE\, \rho'(E)\, \mathcal{E}_{jj}(E, t). \tag{1.5}$$

At zero temperature, $-\rho'$ is a delta function at the Fermi energy and the charge transport is determined by the energy shift at the Fermi energy alone.

There are two noteworthy aspects of this formula. The first one is that $\langle \dot{Q} \rangle$, which is of order ω, can be accurately computed from frozen scattering data which is only an ω^0 approximation. The second one is that the formula holds all the way to $T = 0$, where the adiabatic energy scale ω is large compared to the energy scale T.

As noted above, the matrix of energy shift also determines certain transport properties that are of order ω^2. An example is dissipation at low temperatures. Let $\langle \dot{E} \rangle_j\, (t)$ be the expectation value of energy current in the jth channel. Part of the energy is forever lost as the electrons are dumped into the reservoir. The part that can be recovered from the reservoir, by reclaiming the transported charge, is $\mu \langle \dot{Q} \rangle_j\, (t)$, where μ is the chemical potential. We therefore define the dissipation in a quantum channel as the difference of the two. As we shall show in Section 4.3 the dissipation at $T = 0$ is:[7]

$$\langle \dot{E} \rangle_j\, (t) - \mu \langle \dot{Q} \rangle_j\, (t) = \frac{1}{4\pi}\, (\mathcal{E}^2)_{jj}\, (\mu, t) \geqslant 0. \tag{1.6}$$

[7] For related results on dissipation see, e.g., ref. 28. For relations between dissipation and the S-matrix see ref. 1.

Both the dissipation and the current admit transport formulas that are local in time at $T=0$. Namely, the response at time t is determined by the energy shift at *the same time*. This is remarkable for at $T=0$ quantum correlations decay slowly in time and one may worry that transport at time t will retain memory about the scatterer at early times. This brings us to transport equations which admit a local description only at finite temperatures.

The entropy and noise currents are defined as the difference between the outgoing (into the reservoirs) and incoming entropy (or noise) currents. Namely,

$$\dot{s}_j(t, \mu, T) = \dot{s}(\rho_{\text{out}, j}) - \dot{s}(\rho_j), \qquad \dot{s}(\rho) = \frac{1}{2\pi} \int dE (h \circ \rho)(E, t) \tag{1.7}$$

where[14, 21]

$$h(x) = \begin{cases} -x \log x - (1-x) \log(1-x) & \text{entropy}, \\ x(1-x) & \text{noise}. \end{cases} \tag{1.8}$$

In the adiabatic limit, $\omega \to 0$, and for $\omega \ll T \ll \sqrt{\omega/\tau}$ we find (see Section 4.4)

$$\dot{s}_j(t, \mu, T) = \frac{\beta}{2\pi k} \Delta\mathscr{E}_j^2(\mu, t) \geqslant 0, \qquad k = \begin{cases} 2 & \text{entropy}; \\ 6 & \text{noise}, \end{cases} \tag{1.9}$$

where

$$\Delta\mathscr{E}_j^2 = (\mathscr{E}^2)_{jj} - (\mathscr{E}_{jj})^2 = \sum_{k \neq j} |\mathscr{E}_{jk}|^2. \tag{1.10}$$

When $T \lesssim \omega$ the entropy and noise currents at time t are mindful of the scattering data for earlier times and there are no transport equations that are local in time. What sets them apart from the current and the dissipation is the *non-linear* dependence on the density. The non-linearity makes the transport sensitive to the slow decay of correlations.

Our result about the noise overlap with results that follow from the "full counting statistics" of Levitov *et al.*[24] When there is overlap, the results agree. However, the results are mostly complementary, a reflection of the fact that both the questions and the methods are different. "Counting statistics" determine transport in a *pump cycle* in terms of the *entire history* of the pump. We give information that is local in time. In this sense, we give stronger results. On the other hand, the counting statistics determine *all* moments all the way down to zero temperature, while our results go down to $T=0$ for the current and dissipation but not for the entropy and noise. A detailed comparison of our results with results that follow from the Lesovik–Levitov formalism[24] is made in Appendix B. For other results on noise in pumps see, e.g., ref. 30.

In Section 2 and Appendix A we examine the BPT formula from several perspectives. In Section 2 we consider a pump with two leads where the BPT formula admits an elementary derivation. In Appendix A we derive the BPT formula for an arbitrary number of leads, and show that it can be understood in terms of classical scattering.

Transport in adiabatic scattering is conveniently described using semiclassical methods[25] a.k.a. pseudo-differential (Weyl) calculus.[31] As we shall explain in Section 4, $S(E,t)$ is the principal symbol of the exact S-matrix, S_d. Semi-classical methods can be used to derive Eqs. (1.5)–(1.7). For an alternate point of view using coherent states, see ref. 8.

In Section 6 we discuss the geometric and topological significance of our results. We shall see that charge transport can be formulated in terms of the curvature, or Chern character, of a natural line bundle. This is reminiscent of works of Thouless and Niu[37] which identified quantized charge transport with Chern numbers[38] and inspired the study of quantum pumps. Nevertheless the situation is different here, since the bundle is trivial and, besides, the integration manifold has a boundary. This does not preclude the possibility that charge is quantized for reasons other than being a Chern number. In fact, one can geometrically characterize a class of periodic pump operations[7] for which the transported charge in a cycle, and not just its expectation value, is a non-random integer. It is to be cautioned that a small change of the scattering matrix will typically destroy this quantization.

Some of the results of this paper are new, while others are not. The argument of Section 2 first appeared in ref. 6, and the formulas for energy dissipation and entropy production (Section 5) were derived, non-rigorously, in ref. 7, with supporting estimates on the extent to which $\mathscr{E}_d$ can be approximated by $\mathscr{E}$ appearing in ref. 8. A rigorous proof of the BPT formula, along lines somewhat different from those presented here, appeared in ref. 9. Sections 3, 6, and Appendix A, by contrast, are almost completely new material. By combining old results with new insights, we have attempted to produce a consistent and comprehensive description of quantum pumping.

2. PEDESTRIAN DERIVATION OF BPT

At $T=0$ the Fermi energy is a step function and $\rho'(E) = -\delta(\mu - E)$, and the BPT formula, Eq. (1.5), takes the form

$$\langle \dot{Q} \rangle_j\,(\mu, t) = \frac{1}{2\pi}\,\mathscr{E}_{jj}(\mu, t). \tag{2.1}$$

In this section we shall describe an argument[(6)] that explains this equation in the two channel case. The two channel case is special in that the changes in the scattering matrix break into elementary processes so that for each one BPT follows either from simple physical arguments or from known facts.[8]

In the two channel case, Fig. 1, the frozen, on shell, S-matrix takes the form

$$S(\mu) = \begin{pmatrix} \mathrm{r} & \mathrm{t}' \\ \mathrm{t} & \mathrm{r}' \end{pmatrix}(\mu), \tag{2.2}$$

with r and t (respectively r′ and t′) the reflection and transmission coefficients from the left (right). Equation (2.1) reads

$$2\pi \langle dQ \rangle_- = i(\bar{\mathrm{r}}\,\mathrm{dr} + \bar{\mathrm{t}}'\,\mathrm{dt}'), \qquad 2\pi \langle dQ \rangle_+ = i(\bar{\mathrm{r}}'\,dr' + \bar{\mathrm{t}}\,\mathrm{dt}) \tag{2.3}$$

$\langle dQ \rangle_-$ is made from data $(\mathrm{r}, \mathrm{t}')$ describing the scattering to the left, and similarly $\langle dQ \rangle_+$ from those to the right.[9]

To identify the physical interpretation of the differentials we introduce new coordinates $(\theta, \alpha, \phi, \gamma)$. The most general unitary 2×2 matrix can be expressed in the form:

$$S = e^{i\gamma} \begin{pmatrix} e^{i\alpha}\cos\theta & ie^{-i\phi}\sin\theta \\ ie^{i\phi}\sin\theta & e^{-i\alpha}\cos\theta \end{pmatrix} \tag{2.4}$$

where $0 \leqslant \alpha,\ \phi < 2\pi$, $0 \leqslant \gamma < \pi$, and $0 \leqslant \theta \leqslant \pi/2$. In terms of these parameters, the BPT formula reads

$$2\pi \langle dQ \rangle_{\pm} = \pm(\cos^2\theta)\, d\alpha \mp (\sin^2\theta)\, d\phi - d\gamma. \tag{2.5}$$

As we shall now explain, the variations $d\alpha$, $d\phi$, and $d\gamma$ can be identified with simple physical processes.

[8] We assume that the transported charge depends only on $S(\mu)$ and, linearly, on $dS(\mu)$, regardless of the physical realization of the scatterer.

[9] This is why S^* is on the right in the energy shift, Eq. (1.2).

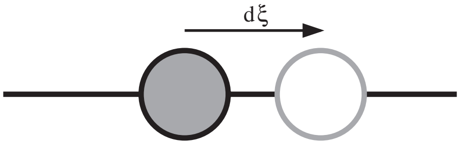

Fig. 2. Moving the scatterer changes $\alpha \to \alpha + 2k_F\, d\xi$.

2.1. The Snowplow

Let k_F be the Fermi momentum associated with μ. Translating the scatterer a distance $d\xi$ multiplies r, (r′) by $e^{2ik_F\, d\xi}$, $(e^{-2ik_F\, d\xi})$, and leaves t and t′ unchanged. It follows that $d\alpha = 2k_F\, d\xi$ corresponds to shifting the scatterer. (See Fig. 2.)

As the scatterer moves, it attempts to push the $k_F\, d\xi/\pi = d\alpha/2\pi$ electrons that occupy the region of size $d\xi$ out of the way, much as a snowplow attempts to clear a path on a winter day. Of these, a fraction $|\mathrm{t}|^2 = \sin^2\theta$ will pass through the scatterer (or rather, the scatterer will pass through them), while the remaining fraction $|\mathrm{r}|^2 = \cos^2\theta$ will be propelled forward, resulting in net charge transport of

$$2\pi \langle dQ \rangle_{\pm} = \pm (\cos^2\theta)\, d\alpha, \tag{2.6}$$

in accordance with Eq. (2.5).

Remark 2.1. It is instructive to examine the special case of a uniformly moving scatterer where we can use Galilei transformations to compute the charge transport exactly. By taking the limit of a slowly moving scatterer we get a check on the result above.

Since the mass of the electron is one, the Galilean shift from the lab frame to the frame of the scatterer shifts each momentum by $-\dot{\xi}$. In the lab frame, the incoming states are filled up to the Fermi momentum k_F while in the moving frame the incoming states of the $\pm$ channels are filled up to momenta $k_F \pm \dot{\xi}$. In the moving frame, the outgoing states on the $\pm$ channels are filled up to $k_F \mp \dot{\xi}$, and partially filled with density $|\mathrm{t}'(k)|^2$ for momenta in the interval $(k_F - \dot{\xi}, k_F + \dot{\xi})$. Transforming back to the lab frame we find for $\delta\rho$ of the $-$ $(=$ left) channel

$$\delta\rho_-(k^2) = \begin{cases} 0 & \text{if} \quad k < k_F - 2\dot{\xi} \\ -|\mathrm{r}'(k+\dot{\xi})|^2 & \text{if} \quad k_F - 2\dot{\xi} < k < k_F \\ 0 & \text{if} \quad k > k_F. \end{cases} \tag{2.7}$$

To order $\dot{\xi}$,

$$\delta\rho_-(E) = -2k_F \dot{\xi}\, |\mathrm{r}'(k_F)|^2\, \delta(E-\mu). \tag{2.8}$$

Since the current is

$$\langle \dot{Q} \rangle_j\, (t) = \frac{1}{2\pi} \int_0^\infty dE\; \delta\rho_j(E, t), \tag{2.9}$$

Eq. (2.6) is reproduced.

Remark 2.2. The net outflow of charge, $\langle dQ \rangle_- + \langle dQ \rangle_+$, vanishes to order $\dot{\xi}$ but not to order $\dot{\xi}^2$. This is because the moving snowplow leaves a region of reduced density in its wake.

2.2. The Battery

To vary ϕ we add a vector potential A. This induces a phase shift $d\phi = \int A$ across the scatterer, and multiplies t, (t′) by $e^{id\phi}$, $(e^{-id\phi})$, while leaving r and r′ unchanged. This phase shift depends only on $\int A$, and is independent of the placement or form of the vector potential. The variation in the vector potential induces an EMF of strength $-\int \dot{A} = -\dot{\phi}$. To first order, the current is simply the voltage times the Landauer conductance $|\mathrm{t}|^2/2\pi$.[21] That is,

$$2\pi \langle dQ \rangle_\pm = \mp\, (\sin^2\theta)\; d\phi, \tag{2.10}$$

in agreement with Eq. (2.5). (See Fig. 3.)

Remark 2.3. Consider the special case of a time independent voltage drop. In a gauge where the battery is represented by a scalar potential, the pump is represented by a time independent scattering problem where the potential has slightly different asymptotes at $\pm\infty$. If the battery is placed to the left of the scatterer, the states of particles incident

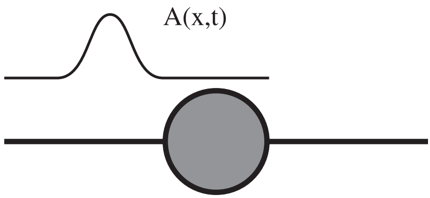

Fig. 3. Applying a vector potential changes $\phi \to \phi + \int A$.

from that side are occupied up to energy $\mu - \dot{\phi}$, while those incident from the right are occupied up to energy μ. Suppose $\dot{\phi}$ is negative. Then $\delta\rho_+$ is

$$\delta\rho_+(E) = \begin{cases} 0 & \text{if} \quad E < \mu, \\ |\mathrm{t}(E)|^2 & \text{if} \quad \mu < E < \mu - \dot{\phi}, \\ 0 & \text{if} \quad E > \mu - \dot{\phi}. \end{cases} \tag{2.11}$$

If, however, the battery is placed to the right of the scatterer then $\delta\rho_+$ is

$$\delta\rho_+(E) = \begin{cases} 0 & \text{if} \quad E < \mu, \\ |\mathrm{t}(E+\dot{\phi})|^2 & \text{if} \quad \mu < E < \mu - \dot{\phi}, \\ 0 & \text{if} \quad E > \mu - \dot{\phi}. \end{cases} \tag{2.12}$$

In either case, to leading order in $\dot{\phi}$,

$$\delta\rho_+(E) = -\dot{\phi}\, |\mathrm{t}(\mu)|^2\, \delta(E-\mu). \tag{2.13}$$

Plugging in Eq. (2.9), we recover Eq. (2.5).

Remark 2.4. To leading order in $\dot{\phi}$, $\delta\rho_+$ is independent of whether the battery is to the left of the pump or to the right of it. To order $\dot{\phi}^2$ this is no longer true as one sees from Eqs. (2.11) and (2.12). The frozen S-matrix is, however, insensitive to the location of the battery. It follows that it is impossible to have a formula for $\delta\rho$, accurate to order $O(\omega^2)$, that involves only the frozen S-matrix and its derivatives (see ref. 29 for some model calculations in the non-adiabatic regime).

2.3. The Sink

The scattering matrix depends on a choice of fiducial points—the choice of an origin for the two channels. Moving the two fiducial points out a distance $d\xi$ may be interpreted as forfeiting part of the channels in favor of the scatterer. This new, bigger, scatterer is shown schematically in Fig. 4. This transforms the scattering matrix according to

$$S(k_{\mathrm{F}}) \to e^{id\gamma}\, S(k_{\mathrm{F}}), \qquad d\gamma = 2k_{\mathrm{F}}\, d\xi. \tag{2.14}$$

This operation removes $k_{\mathrm{F}}\, d\xi/\pi$ electrons from each channel and so we get

$$2\pi\langle dQ\rangle_{\pm} = -2k_{\mathrm{F}}\, d\xi = -d\gamma, \tag{2.15}$$

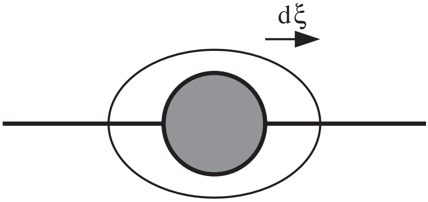

Fig. 4. A scatterer that has gobbled up $d\xi$ of each wire.

in accordance with Eq. (2.5). Changing γ is therefore equivalent to having the pump swallow particles from the reservoirs.

For arbitrary variations dS the above result still holds for the sum $dQ_- + dQ_+$. This follows directly from a fact in scattering theory known as Birman–Krein formula[39] and in physics as Friedel sum rule[19] which says that the excess number of states below energy μ associated with the scatterer is $(2\pi i)^{-1} \log \det S(\mu)$, whence

$$-2\pi(\langle dQ\rangle_- + \langle dQ\rangle_+)(\mu) = -id \log \det S(\mu) = 2\, d\gamma. \tag{2.16}$$

2.4. The Ineffective Variable

We have already seen that changes in α, ϕ, γ yield transported charges $dQ_\pm$ which are correctly reproduced by Eq. (2.5). Moreover, for any change of S, the sum $\langle dQ\rangle_- + \langle dQ\rangle_+$ is correctly described as well. To complete the derivation of Eq. (2.5) we must consider variations in θ, with α, ϕ, and γ fixed, and show that $\langle dQ\rangle_- - \langle dQ\rangle_+ = 0$.

Suppose a scatterer has α, ϕ, and γ fixed, but θ changes with time. By adding a (fixed!) vector potential and translating the system a (fixed!) distance,[10] we can assume that $\alpha = \phi = 0$. Now imagine a second scatterer that is the mirror image of the first (i.e., with right and left reversed) as in Fig. 5. Since θ and γ are invariant under right-left reflection, and since α and ϕ are odd under right-left reflection, the second scatterer has the same frozen S matrix as the first, and this equality persists for all time.

From the frozen scattering data we therefore conclude that the currents for the second system are the same as for the first. However, by reflection symmetry, $\langle dQ\rangle_- - \langle dQ\rangle_+$ for the first system equals $\langle dQ\rangle_+ - \langle dQ\rangle_-$ for the second. We conclude that $\langle dQ\rangle_+ - \langle dQ\rangle_- = 0$ for variations of θ.

[10] This can be achieved, in general, only at a fixed energy, and we pick the energy to be the Fermi energy μ.

Fig. 5. An asymmetric scatterer and its image under reflection.

3. TIME DEPENDENT SCATTERING AND WEYL CALCULUS

3.1. The Energy Shift

In this section we describe the notion of energy shift in the context of time dependent scattering theory and derive an operator identity relating the outgoing density ρ_{out} to the incoming density and the energy shift. In Section 4 we then use this identity to derive formulas for the energy dissipation, noise, and entropy production.

The (exact, dynamical) S-matrix is a comparison between the dynamics generated by a reference time-independent Hamiltonian H_0 (often called the free Hamiltonian), and the actual time-dependent Hamiltonian $H(t) = H_0 + V(t)$. Let $U(t_2, t_1)$ be the time-evolution from time t_1 to time t_2, generated by $H(t)$, and let $U_0(t_2, t_1) = e^{-i(t_2 - t_1) H_0}$ be the time-evolution generated by H_0. The S-matrix is defined to be

$$S_d(t) = \lim_{t_\pm \to \pm\infty} U_0(t, t_+)\, U(t_+, t_-)\, U_0(t_-, t), \tag{3.1}$$

assuming the limit exists.

Energy is conserved in time independent scattering but not in time dependent scattering. In the time independent case, conservation of energy is expressed as the statement that the scattering matrix S commutes with H_0 (not H!). Hence, for the frozen S-matrix

$$S_f e^{-iH_0 t} = e^{-iH_0 t} S_f. \tag{3.2}$$

This may be interpreted as the statement that the state ψ, and the time shifted state $e^{-iH_0 t}\psi$ both see the same scatterer. Therefore it makes no difference if the time shift takes place before or after the scattering.

This is, of course, not true in the time-dependent case. The states ψ and its time shift $e^{-iH_0 t}\psi$ do not see the same scatterer, and the (dynamical) scattering matrix S_d acquires a time dependence:

$$S_d(t)\, e^{-iH_0 t} = e^{-iH_0 t} S_d(0). \tag{3.3}$$

In the time dependent case one does not have a single scattering matrix, but rather a family of operators $S_d(t)$. Since these operators are all related by conjugation, any one of them is unitarily equivalent to any other. To pick one is to pick a reference point on the time axis. We shall henceforth write $S_d(0)$ as simply S_d.

If $S_d(t)$ is unitary,[11] which we henceforth assume, then $\mathscr{E}_d(t) = i\dot{S}_d(t)\, S_d^*(t)$ is Hermitian. Taking the derivative of (3.3), we obtain the equation of motion

$$i\dot{S}_d(t) = [H_0, S_d(t)]. \tag{3.4}$$

Using the (assumed) unitarity of S_d, this can be reorganized as

$$S_d(t)\, H_0 S_d^*(t) = H_0 - \mathscr{E}_d(t). \tag{3.5}$$

Conjugation by the scattering matrix takes outgoing observables to incoming observables. Equation (3.5) justifies identifying $\mathscr{E}_d$ with the operator of energy shift.

Remark 3.1. If we let $Q_j(t)$ denote the projection on the states in the jth channel, then $\hat{Q}_j(t) = S_d Q_j(t)\, S_d^*$ projects on the outgoing states fed by the jth channel. The energy shift generates the evolution of $\hat{Q}_j$:

$$i\dot{\hat{Q}}_j = [\mathscr{E}_d, \hat{Q}_j]. \tag{3.6}$$

We are now ready to derive Eq. (1.1), which is an operator identity for ρ_{out}. This is our starting point in analyzing adiabatic transport. By the functional calculus we can extend Eq. (3.5), evaluated at $t = 0$, to (measurable) functions of H_0, namely

$$\rho_{\text{out}} = S_d\, \rho(H_0)\, S_d^* = \rho(H_0 - \mathscr{E}_d). \tag{3.7}$$

This identity is exact, and does not assume an adiabatic time dependence. In the adiabatic limit, however, we may approximate the energy shift operator $\mathscr{E}_d$, acting on states of energy E and approximate time of passage t, with the matrix of energy shift $\mathscr{E}(E, t)$. This is done in Section 4. Having obtained ρ_{out} in terms of $\mathscr{E}(E, t)$, we can then compute dissipation, noise, and entropy production.

Remark 3.2. For comparison we establish the classical counterpart to Eq. (3.5). Let Γ be the classical phase space described in Appendix A.2

[11] $S_d(t)$ is unitary as a map between the spaces of in and out states which may differ because states may get trapped or released from the pump.

and let $\phi_s \colon \Gamma \to \Gamma$ be the flow $\phi_s(E, t) = (E, t - s)$ generated by the Hamiltonian $h(E, t) = E$, i.e., the solution of the canonical equations of motion

$$\frac{d}{ds} \phi_s(x) = I(dh)|_{\phi_s(x)}, \tag{3.8}$$

where $x = (E, t)$ and $I \colon T^*\Gamma \to T\Gamma$ is the symplectic 2-form. If times of passage are measured not w.r.t. time 0 but w.r.t. time t, then the scattering map, $S_d(t)$, satisfies, cf. Eq. (3.3),

$$S_d(t) \circ \phi_t = \phi_t \circ S_d, \tag{3.9}$$

where $S_d(0) = S_d$ has been introduced in Eq. (A.10). Since $S_d(t)$ is a family of symplectic maps its vector field is Hamiltonian:

$$\frac{d}{dt} S_d(t)(x)|_{t=0} = I(d\mathscr{E}_d)|_{S_d(x)}, \tag{3.10}$$

where $\mathscr{E}_d$ is a function on Γ uniquely determined up to an additive constant. By taking derivatives of (3.9) at $t = 0$ we obtain $I(d\mathscr{E}_d) + S_{d^*}(I(dh)) = I(dh)$. Since S_d is symplectic we have $S_{d^*}I = I$ and hence $S_{d^*}(I(dh)) = (S_{d^*}I)(S_{d^*}\, dh) = I(S_d^*)^{-1}\, dh = Id(h \circ S_d^{-1})$, so that we conclude

$$h \circ S_d^{-1} = h - \mathscr{E}_d, \tag{3.11}$$

provided the constant not determined by S_d is properly adjusted.

3.2. The Weyl Calculus

A convenient language for discussing the relation between operators in quantum mechanics and functions on phase space, called symbols, is the Weyl calculus.[25, 31] For pumps the classical phase space is described at the beginning of Appendix A.2, with points labelled by the pair (E, t), where E is the energy of the (classical) particle and t its time of passage at the origin. An additional index $j = 1, \ldots, n$ labels the channels.

The relation of a (matrix valued) symbol $a(E, t)$ to the corresponding operator A is

$$\langle t, j| \, A \, |t', j'\rangle = \frac{1}{2\pi} \int dE \, e^{-i(t-t')\,E} a_{jj'}\left(E, \frac{t+t'}{2}\right), \tag{3.12}$$

where $|t, j\rangle$ is the (improper) state in the jth channel whose time of passage at the scatterer (in the H_0 dynamics) is t. Equivalently,

$$\langle E, j| \, A \, |E', j'\rangle = \frac{1}{2\pi} \int dt \, e^{i(E-E')\,t} a_{jj'}\left(\frac{E+E'}{2}, t\right), \tag{3.13}$$

where $|E, j\rangle$ is the (improper) state in the $j$the channel with energy E. It follows that (if A is trace class[34])

$$\mathrm{Tr}\, A = \frac{1}{2\pi} \int \mathrm{tr}\, a\, dE\, dt \tag{3.14}$$

where tr a denotes a trace over channels, i.e., a trace of finite dimensional matrices. Similarly, if a or b are (locally supported) functions, we have

$$\mathrm{Tr}(AB) = \frac{1}{2\pi} \int \mathrm{tr}(ab)\, dE\, dt. \tag{3.15}$$

4. ADIABATIC TRANSPORT

The notion of approximation in adiabatic scattering requires some explanation. In this regime the scattering of a particle occurs on the time scale of the dwell time τ which is short compared to the adiabatic time scale ω^{-1}. Therefore, the (unitary) operator S_d should be related to the frozen scattering matrices $S(E, t)$. While the uncertainty relation forbids specifying both coordinates E and t of a particle, the variables on which $S(E, t)$ actually depends are E and ωt. This gives adiabatic scattering a semiclassical flavor where ω plays the role of $\hbar$. Its theory can be phrased in terms of the Weyl calculus[25, 31] with symbols which are power[12] series in ω. In particular, as we shall explain, $S(E, t)$ may be interpreted as the principal symbol of S_d. The chain of argument in making the identification goes through the frozen S-matrix, $S_f(t)$, where the time of freezing, t, is picked by the incoming state.

4.1. Adiabatic Scattering

We shall show the following correspondence between operators and symbols which, in our case, are $n \times n$ matrix functions of E and t:

$$S_d(t_0) \Leftrightarrow S(E, t+t_0) + O(\omega) \tag{4.1}$$

$$\mathscr{E}_d \Leftrightarrow \mathscr{E}(E, t) + O(\omega^2) \tag{4.2}$$

$$\rho_{\mathrm{out}} \Leftrightarrow \rho(E) - \rho'(E)(\mathscr{E}(E, t) + O(\omega^2)) + \tfrac{1}{2}\, \rho''(E)\, \mathscr{E}^2(E, t) + O(\omega^3). \tag{4.3}$$

[12] The dimensionless expansion parameter is $\omega\tau$.

Since the Fermi function at $T=0$ is a step function, ρ' is a delta function and consequently, the notion of smallness in the expansion in Eq. (4.3) is in the sense of distributions.[13]

To see the first relation, let $|t, j\rangle$ denote the state that traverses the scatterer at time t and $S_f(s)$ denote the frozen S-matrix associated with the Hamiltonian in effect at time s. Then

$$\langle t, j|\, S_d\, |t', j'\rangle = \left\langle t, j \left|\, S_f\left(\frac{t+t'}{2}\right) \right| t', j' \right\rangle + O(\omega). \tag{4.4}$$

The matrix elements on both sides are significant provided $t-t'$ is small, within the order of the dwell time, or the Wigner time delay. Using

$$|t, j\rangle = (2\pi)^{-1/2} \int dE\, e^{iEt}\, |E, j\rangle \tag{4.5}$$

one finds

$$\langle t, j|\, S_f(s)\, |t', j'\rangle = \frac{1}{2\pi} \int dE\, e^{-i(t-t')\,E}\, S(E, s), \qquad s = \frac{t+t'}{2}, \tag{4.6}$$

and we have used the fact that S_f is energy conserving. This establishes Eq. (4.1) for $t_0=0$ by comparison with Eq. (3.12). The "quantization" of $S(E, t)$ then satisfies Eq. (3.3), as it must.

Equations (4.2) and (4.3) now follow from the rules of pseudo-differential calculus,[(31)] and the operator identity for the outgoing states Eq. (1.1).

4.2. Currents

We shall here present a formal, but relatively straightforward derivation of BPT using Weyl calculus.

Let $Q_j^{\mathrm{in/out}}(x, t_0)$ be the observable associated with counting the incoming/outgoing particles in a box that lies to the right of a point x in the jth channel at the point in time t_0. The point x is chosen far from the scatterer, but not so far that the time delay relative to the pump is of order ω^{-1}. Namely, $v\tau \ll x \ll v/\omega$. The symbol of $Q^{\mathrm{in/out}}$ is a matrix valued step function:

$$Q_j^{\mathrm{in/out}}(x, t_0) \Leftrightarrow P_j \theta(v(t_0-t)-x)\, \theta(\mp(t_0-t)), \qquad (P_j)_{ik} = \delta_{jk}\delta_{ij}, \quad v = \epsilon'(p), \tag{4.7}$$

[13] In agreement with Eqs. (2.8) and (2.13).

and P_j is the projection matrix on the jth channel. Indeed, the position of a particle with coordinates (E, t) at time 0 will be $-v(t-t_0)$ at time t_0, see Eq. (A.9). The particle will then be outgoing if $t-t_0<0$. Notice that $t=t_0$ falls outside of the support of the first Heaviside function. The associated incoming/outgoing current operators are

$$\dot{Q}_j^{\mathrm{in/out}}(x, t_0)=i[H, Q_j^{\mathrm{in/out}}(x, t_0)]=i[H_0, Q_j^{\mathrm{in/out}}(x, t_0)]. \tag{4.8}$$

Here we used the fact that beyond x, deep inside the channel, $H(t)$ coincides with H_0. The symbol associated with the current is most easily computed recalling that in Weyl calculus commutators are replaced by Poisson brackets. This reproduces the usual notion of a current

$$\dot{Q}_j^{\mathrm{in/out}}(x, t_0) \Leftrightarrow P_j\{E, \theta(v(t-t_0)-x)\}=\mp P_j\, \delta(t-t_0-x/v)\, \theta(\mp(t_0-t)), \tag{4.9}$$

x is where the "ammeter" is localized. By the assumption that the ammeter is not too far it leads to a slight modification of t_0, the time when current is measured. We henceforth drop x. Now the expectation value of the current is

$$\langle\dot{Q}\rangle_j\, (x, t_0)=\mathrm{Tr}(\rho_{\mathrm{out}} Q_j^{\mathrm{out}})+\mathrm{Tr}(\rho Q_j^{\mathrm{in}})=\mathrm{Tr}(\delta\rho\, \dot{Q}_j^{\mathrm{out}}(x, t_0)), \quad \delta\rho=\rho_{\mathrm{out}}-\rho. \tag{4.10}$$

Using Eq. (3.15) to evaluate the trace we find

$$\begin{aligned}\langle\dot{Q}\rangle_j\, (x, t_0) &= -\frac{1}{2\pi}\int dE\, dt\, \rho'(E)\, \mathscr{E}_{jj}(E, t)\, \delta(t-t_0)+O(\omega^2)\\ &= -\frac{1}{2\pi}\int dE\, \rho'(E)\, \mathscr{E}_{jj}(E, t_0)+O(\omega^2)\end{aligned} \tag{4.11}$$

reproducing Eq. (1.5).

4.3. Dissipation

To compute the dissipation we start as in the previous section. Let $D_j^{\mathrm{in/out}}$ denote the observable associated with the incoming/outgoing excess energy in the jth channel in a box to the right of the point x. The excess energy is, of course, energy measured relative to the Fermi energy:

$$D_j^{\mathrm{in/out}}(x, t_0)=\tfrac{1}{2}\,\{Q_j^{\mathrm{in/out}}(x, t_0), H_0-\mu\} \tag{4.12}$$

and $Q_j^{\text{in/out}}$ is as in Eq. (4.7). The observable associated with dissipation current in the jth channel is the time derivative of the excess energy, i.e.,

$$\dot{D}_j^{\text{in/out}}(x, t_0) = \dot{E}_j^{\text{in/out}}(x, t_0) - \mu \dot{Q}_j^{\text{in/out}}(x, t_0) = i[H_0, D_j^{\text{in/out}}(x, t_0)]. \quad (4.13)$$

The symbol corresponding to the dissipation current is then

$$D_j^{\text{in/out}}(x, t_0) \Leftrightarrow \mp P_j(E-\mu)\, \delta(t - t_0 - x/v)\, \theta(\mp(t_0 - t)). \quad (4.14)$$

The expectation value of the dissipation current is therefore

$$\langle \dot{D} \rangle_j\, (x, t_0) = \operatorname{Tr}(\delta\rho\, \dot{D}_j^{\text{out}}(x, t_0)). \quad (4.15)$$

We shall now show that for $T \lesssim \sqrt{\omega/\tau}$ the dissipation is quadratic in ω and is determined by Eq. (1.6).

As in Section 4.2 we shall evaluate the trace using Eq. (3.15). At low temperature ρ' is concentrated near the Fermi energy. We may then approximate the energy shift up to its linear variation near μ. For the term proportional to ρ' in the expansion Eq. (4.3) the contribution to the dissipation is proportional to

$$\begin{aligned} -\frac{1}{2\pi} \int dE\, \rho'(E)(\mathscr{E}_{jj}(\mu, t_0) + (E-\mu)\, \mathscr{E}'_{jj}(\mu, t_0) + O(\omega^2))(E-\mu) \\ = O(\beta e^{-\beta\mu}) + O(\omega T^2) + O(\omega^2 T). \end{aligned} \quad (4.16)$$

The term proportional to ρ'' in the expansion gives,

$$\frac{1}{4\pi} \int dE\, \rho''(E)(\mathscr{E}^2)_{jj}\, (E, t_0)(E-\mu) = \frac{1}{4\pi} (\mathscr{E}^2)_{jj}\, (\mu, t_0) + O(\omega^2 T), \quad (4.17)$$

which is the requisite result, Eq. (1.6).

The result (1.6) is remarkable in that we obtain the dissipation to order ω^2 by making two approximations, each valid only to order ω. First we replace $\mathscr{E}_d$ with $\mathscr{E}$, and then we evaluate $\mathscr{E}$ at $E = \mu$. Had we used this procedure to compute the quantities $\dot{E}_j$ and $\dot{Q}_j$ separately, each of them would be off by nonzero $O(\omega^2)$ terms (as can be seen in the snowplow and battery examples); nevertheless, the combination $\dot{E}_j - \mu \dot{Q}_j$ is computed correctly to order ω^2. The reason is that in each quantum channel one has the following lower bound on the dissipation:[7]

$$\dot{E}_j - \mu \dot{Q}_j \geqslant \pi \dot{Q}_j^2. \quad (4.18)$$

This bound is saturated by the outgoing population distribution that is filled up to energy μ and empty thereafter. The dissipation should therefore be quadratic in the deviation of the outgoing distribution from this minimizer. Since the outgoing distribution is an $O(\omega)$ perturbation of the minimizer, knowing the distribution to order ω should give the dissipation to order ω^2.

Remark 4.1. There would appear to be two problems with the argument above. In minimizing a functional on a region with a boundary, one obtains a quadratic estimate for the functional around its minimizer if the minimum occurs at an interior point. If the minimum occurs at the boundary, then a variation away from the boundary can increase the function to first order. Furthermore, whether the minimum occurs at an interior point or on the boundary, quadratic estimates depend on the Hessian being a bounded operator. If the Hessian is unbounded, then an arbitrarily small change in the point can cause an arbitrarily large increase in the functional. In our case, the minimum occurs at a point that is on the boundary of the constraints $0 \leqslant \rho(E) \leqslant 1$. There are large modes for the Hessian, involving adding electrons at arbitrarily high energies.

Fortunately, neither exception is relevant. In fact, the correction of the distribution, as given by (4.3), consists of a local reshuffling of electrons around the Fermi energy and does not involve the large modes of the Hessian. These variations should not be viewed as being either towards or away from the boundary, since neither the expression (3.7) nor its opposite (replacing $\mathscr{E}$ with $-\mathscr{E}$) violates the constraints.

4.4. Entropy and Noise Currents

Entropy and noise introduce a new element in that the transport equation, Eq. (1.7), depends on the density through a *non-linear* function $h(\rho)$. For the entropy and noise $h(x)$ is given in Eq. (1.8). Using the fact that in either case $h(0) = h(1) = 0$, we shall show that for $\omega \ll T \ll \sqrt{\omega/\tau}$ the currents are quadratic in ω and are given by

$$\dot{s}_j(t, \mu, T) = \frac{\beta}{2\pi} \Delta\mathscr{E}_j^2(\mu, t)) \int_0^1 dx\, h(x), \tag{4.19}$$

where $\Delta\mathscr{E}_j^2$ has been defined in Eq. (1.10). For the entropy the integral gives $1/2$ and for the noise it gives $1/6$. To complete the derivation of the noise and entropy currents, we now derive Eq. (4.19).

The condition $\omega \ll T$ makes it possible to consider the outgoing state of the electrons with a fixed time of passage, provided the time resolution is short compared to ω^{-1} but large w.r.t. T^{-1}. The state $\rho_{\text{out}, j} = P_j \rho_{\text{out}} P_j$ is then given, see (4.3), as

$$\rho_{\text{out}, j}(E) = \rho(E - \mathscr{E}_{jj}(E, t)) + \tfrac{1}{2} \rho''(E)((\mathscr{E}^2)_{jj}\,(E, t) - \mathscr{E}_{jj}(E, t)^2). \qquad (4.20)$$

The entropy/noise current (1.7) is

$$\frac{1}{2\pi} \int dE((h \circ \rho)(E - \mathscr{E}_{jj}(E, t)) - (h \circ \rho)(E))$$
$$+ \frac{1}{4\pi} \int dE(h' \circ \rho)(E)\, \rho''(E)\, \Delta\mathscr{E}_j^2(E, t). \qquad (4.21)$$

In these integrals, $\mathscr{E}_{jj}$ may be regarded as constant in E because of the condition $T \ll \sqrt{\omega/\tau}$. The first integral then vanishes and in the second we may pull $\Delta\mathscr{E}_j^2(\mu, t)$ out of the integral. This leaves us with the integral

$$\int dE(h' \circ \rho)(E)\, \rho''(E) = -\beta \int_0^1 d\rho\, h'(\rho)(1 - 2\rho)$$
$$= 2\beta \int_0^1 d\rho\, h(\rho), \qquad (4.22)$$

where, in the second step, we have used a property of the Fermi function, $\rho' = -\beta\rho(1-\rho)$, and an integration by parts in the last step. This establishes the result.

We have nothing to say about the range $T \lesssim \omega$. The noise at $T = 0$ can be calculated using a formalism of Lesovik and Levitov that we discuss in the appendix. This formula is nonlocal in time. It is instructive to examine what goes wrong with our approach at $T = 0$. In this limit ρ' and ρ'' are distributions and ρ a discontinuous function. Since it is not allowed to multiply distributions by distributions, or even by discontinuous functions, equations such as Eq. (4.22) which are not linear in ρ make no sense. This is a reflection of the fact that in the regime where $T \lesssim \omega$ entropy and noise currents have a memory that goes back in times of order β. In the regime we consider $\omega \ll T$ the memory is short compared with the time scale of the pump and instantaneous formulas make sense. At the opposite regime, where $T \lesssim \omega$, a local formula in time cannot be expected.

5. EXAMPLES

Quantum pumps may be viewed either as particle pumps or as wave pumps. The particle interpretation has a classical flavor where the driving mechanism is identified with forces on the particles. The wave interpretation stresses the role played by phases and suggests that interference phenomena play a role. This duality can be seen in the BPT formula in the two channel case of Section 2. On the one hand Eq. (2.5) makes it clear that the phases in the S-matrix, (α, ϕ, γ), play a role in charge transport. In fact, changing the transmission and reflection probabilities while keeping the phases fixed cannot drive a current. At the same time, the rate of change of two of the three phases, $\dot{\phi}$ and $\dot{\alpha}$, also admit a classical interpretation as EMF and Galilean shift. The pedestrian derivation is a reflection of the fact that particle interpretation is more intuitive. Here we shall consider two examples where dual reasoning is insightful.

5.1. The Bicycle Pump

In an ordinary bicycle pump the action of the valves is synchronized with the motion of the piston. The analogous quantum pump has synchronized gates as shown in Fig. 6. The particle interpretation of the pump is simple and intuitive. The wave (or BPT) point of view is more subtle. In particular as we shall see, in terms of the elementary processes described in Section 2 the pump operates by changing the phases γ and α: Galilean shifts arise from the synchronized action of the gates.

Let us choose a length scale so that $k_F = \pi$ and an energy scale so that $\mu = 1$. In these units, choose the length of the pump, L, to be an integer $L = n$, pick the valves thin, $\delta \ll 1$, and impenetrable, i.e., of height M with $M\delta \gg 1$. Consider the potential, shown in Fig. 6, that depends on two parameters, a and b, that vary on the boundary of the unit square $[0, 1] \times [0, 1]$:

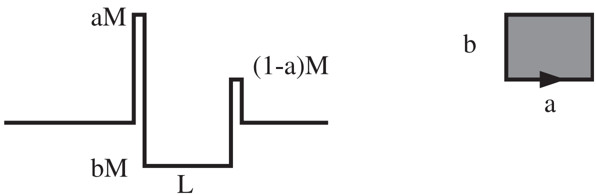

Fig. 6. On the left a typical configuration of the potential of the quantum bicycle pump. On the right a loop in the a–b parameter space.

$$V_{a,b}(x) = \begin{cases} 0 & \text{if} \quad x < 0, \\ aM & \text{if} \quad 0 \leqslant x < \delta, \\ 10b & \text{if} \quad \delta \leqslant x < L, \\ (1-a)\,M & \text{if} \quad L \leqslant x < L+\delta, \\ 0 & \text{if} \quad x \geqslant L+\delta. \end{cases} \tag{5.1}$$

Since the quantum box was designed to accommodate n particles, the pumps transfers n particles in each cycle. Like in the bicycle pump, at all times, at least one of the valves is closed. This give the particle point of view.[14]

We now consider this pump from the perspective of the phases in BPT. At all stages of the cycle, the transmission coefficients at the Fermi energy are essentially zero, so, by unitarity, the reflection coefficients r and r′ are unit complex numbers. The phases of the reflection amplitude, $\gamma \pm \alpha$ of Eq. (2.4), must therefore change by $\pm 2\pi n$ in each cycle of the pump. How does this happen? As we shall see in spite of the fact that the pump is operated by manipulating gate voltages, the interpretation in terms of the S-matrix is in terms of an interplay between Galilean shifts $d\alpha$ and the Birman–Krein term $d\gamma$.

At $a=0$, $b=1$, we have $\mathrm{r}=-1$, since the piston imposes a Dirichlet condition at $x=0$, and $\mathrm{r}' = -\exp(2ik_{\mathrm{F}}L) = -1$, since the valve on the right imposes a Dirichlet condition at $x=L$. As b is decreased, r′ remains -1 (since the right valve is closed) and by Eq. (2.4) $d\alpha = d\gamma$. Meanwhile, the wave functions of incoming waves from the left penetrate deeper and deeper into the region $0 < x < L$, eventually accumulating n half-wave-lengths. The phase of r increases by $2\pi n$, since the left barrier has been effectively shifted a distance L to the right and $\int dQ_1 = -n$.

The path with $b=0$ has no effect on the scattering matrix, since L is an integral number of half-wavelengths, so a Dirichlet condition at $x=0$ is equivalent to a Dirichlet condition at $x=L$. The left valve closes and the right valve opens but no current flows. The remaining two legs of the path can be similarly analyzed. Increasing b with $a=1$ decreases the phase of r′ by $2\pi n$, while decreasing a with $b=1$ has no effect on r or r′.

The fact that $\mathrm{t}=\mathrm{t}'=0$ throughout the process might seem strange. After all, how can you transport particles without transmission? However, this is exactly what happens with classical pumps. A good pump has valves that do not leak.

[14] For related results see, e.g., ref. 23.

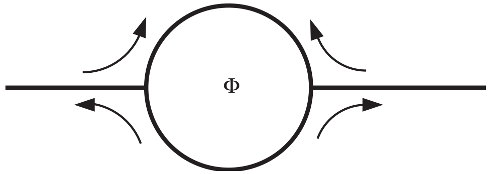

Fig. 7. The graph associated with a model of the quantum Hall effect.

5.2. The U-Turn Pump

The U-turn pump, shown in Fig. 7, is a highly schematic version of the quantum Hall pump. There are two leads connected to a loop of circumference ℓ. The loop is threaded by a slowly varying flux tube carrying a flux Φ. The particle satisfies the free Schrödinger equation on the edges of the graph and and satisfies an appropriate boundary condition at the vertices. The boundary conditions are such that at the Fermi energy all particles are forced to make a U-turn at the loop. Namely, all particles coming from the right circle the loop counter-clockwise and the exit on the right while all those coming from the left circle the loop clockwise and exit on the left.

Let us first look at this pump as a wave pump. Since all particles make a U-turn, the transmission amplitude vanish and the reflection amplitudes are phases. A left mover on the loop accumulates a Bohm–Aharonov phase in addition to the phase due to the "optical length" of the path. This means that the S-matrix at the Fermi energy is

$$S(\mu, \Phi) = \begin{pmatrix} e^{i(k_F\ell+\Phi)} & 0 \\ 0 & e^{i(k_F\ell-\Phi)} \end{pmatrix}. \tag{5.2}$$

By BPT the charge transport is

$$\langle dQ \rangle_{\pm} (\mu) = \pm \frac{d\Phi}{2\pi}. \tag{5.3}$$

One charge is pumped from left to right in a cycle of the pump as Φ increases by 2π, the unit of quantum flux.

The scattering calculation, although easy, does not really explain how the pump operates: How does it transport charges from right to left if all charges are forced to make a U-turn at the loop? The particle interpretation demystifies the pump: Particles in the loop see a force associated with the EMF $\dot{\Phi}$ which make the clockwise movers feel as if they are going uphill while the counter-clockwise movers all go downhill. Because of this

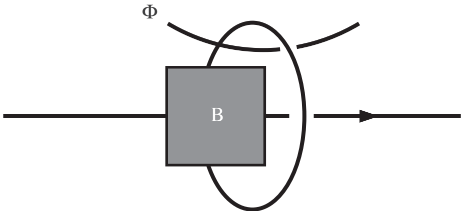

Fig. 8. The Hall effect as a pump driven by the EMF $\dot{\Phi}$.

some of the slow counter-clockwise movers turn into clockwise movers and exit on the other side. Although insightful, the particle interpretation does not readily translate to a qualitative computation without invoking some wave aspects.

The integer quantum Hall effect[17] 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 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. 8.

The U-turn pump of Fig. 7 models the essential features of this geometry. The 2D electron gas in the Hall sample, and the magnetic field applied to the Hall crystal, are modelled by the vertices, which scatter particles in a time-asymmetric manner. The clockwise movers of Fig. 7 correspond to electrons that enter the Hall bar 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 counter-clockwise movers correspond to electrons that go from east to north (along the Hall bar) to south (along the loop) and then to east and out the east lead. By standard arguments,[20] the edge states reflect the existence of localized bulk states in the crystal.

5.3. A Family of Optimal Pumps

Optimal pumps[7] saturate the bound in Eq. (4.18). In ref. 4 it was shown that optimal pumps that do not break time-reversal are transmissionless. (The two examples above also fall into the category of being optimal and transmissionless.) We recall that under time-reversal S is mapped to $\overline{S^{-1}} = S^t$ (assuming that the operation does not act on the channel indices). If invariant, S has symmetric transmission coefficients. The question was posed in ref. 4 whether an optimal pump, which is not time-reversal invariant, could be constructed. The following example shows that such an optimal pump can have any value of r and t.

In the battery of Section 2.2 the scatterer got in the way of the electrons, and the most efficient transport was with $r=0$. In the snowplow of Section 2.1 the scatterer pushed the electrons and the most efficient transport was with $|r|=1$. In the following example of optimal pump we combine a voltage with a moving scatterer, such that the scatterer is moving along with the electrons, neither pushing nor getting in the way. In this case, the scatterer doesn't actually *do* anything, and we get efficient transport, regardless of the initial values of (r, t, r', t').

Write the scattering matrix of a system where $\alpha = 2\mu\xi$ and ϕ evolve as

$$S(\mu) = \begin{pmatrix} re^{-2i\mu\xi} & t'e^{-i\phi} \\ te^{i\phi} & r'e^{2i\mu\xi} \end{pmatrix}. \tag{5.4}$$

Synchronizing the velocity $\dot{\xi}$ with the voltage $\dot{\phi}$ according to

$$2\mu\dot{\xi} = \dot{\phi} \tag{5.5}$$

makes $\dot{S} = i\dot{\phi}\sigma_3 S$. The energy shift is then a diagonal matrix

$$\mathcal{E} = i\dot{S}S^* = -\dot{\phi}\sigma_3 \tag{5.6}$$

which implies that the pump is optimal.

5.4. The Phase Space of a Snowplow

We give a description of a classical snowplow moving on the real axis at speed v_0 during the time interval $[-T, T]$, but at rest before and after that. It is described by the (total) phase space $\mathbf{R}^2 \ni (x, p)$ with Hamiltonian function $h = p^2/2 + V(t)$, where $V(t)$ is a barrier of fixed height $V > v_0^2/2$ and zero width located at

$$x(t) = \begin{cases} -v_0 T, & (t \leqslant -T), \\ v_0 t, & (-T < t < T), \\ v_0 T, & (t \geqslant -T). \end{cases} \tag{5.7}$$

We use the notation of Appendix A.2 and denote by 1 the left channel $(x < 0)$ and by 2 the right one $(x > 0)$. Let $\Gamma_{ij}^+ \subset \Gamma_j \subset \Gamma^+$ be the outgoing labeled trajectories originating from channel i and eventually ending in channel j. The same meaning has $\Gamma_{ij}^- \subset \Gamma_i \subset \Gamma^-$, except that the trajectories are incoming labeled.

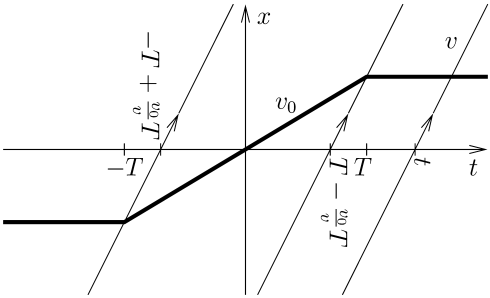

Fig. 9. The thick line represents the position $x(t)$ of the snowplow. The other lines are free trajectories of common energy E indicated by the slope $v=\sqrt{2E}>0$. Their times of passage t are read off at the intercepts with the abscissa.

If a particle crosses the above scatterer of zero width, then its trajectory is free at all times. Hence

$$\Gamma_{12}^{-}=\Gamma_{12}^{+}, \qquad \Gamma_{21}^{-}=\Gamma_{21}^{+}. \tag{5.8}$$

It suffices to compute these subsets only. The remaining ones are then given by complementarity:

$$\Gamma_{i1}^{-}\cup\Gamma_{i2}^{-}=\Gamma_{i}, \qquad \Gamma_{1j}^{+}\cup\Gamma_{2j}^{+}=\Gamma_{j}, \tag{5.9}$$

with disjoint unions.

- $\Gamma_{12}^{-}=\Gamma_{12}^{+}$. Depending on their time of passage t, trajectories of this type will (see Fig. 9) require an energy $E=v^2/2>E_c\equiv v_c^2/2$, with critical energy E_c given as

$$E_c=V \qquad \text{if} \quad |t|>T-\frac{v_0}{v}T=T-\frac{v_0}{\sqrt{2E}}T;$$

resp. by $v_c-v_0=\sqrt{2V}$, i.e.,

$$E_c=\frac{1}{2}(\sqrt{2V}+v_0)^2 \qquad \text{if} \quad |t|\leqslant T-\frac{v_0}{\sqrt{2E}}T.$$

This portion of phase space is drawn dark shaded in the upper part of Fig. 10.

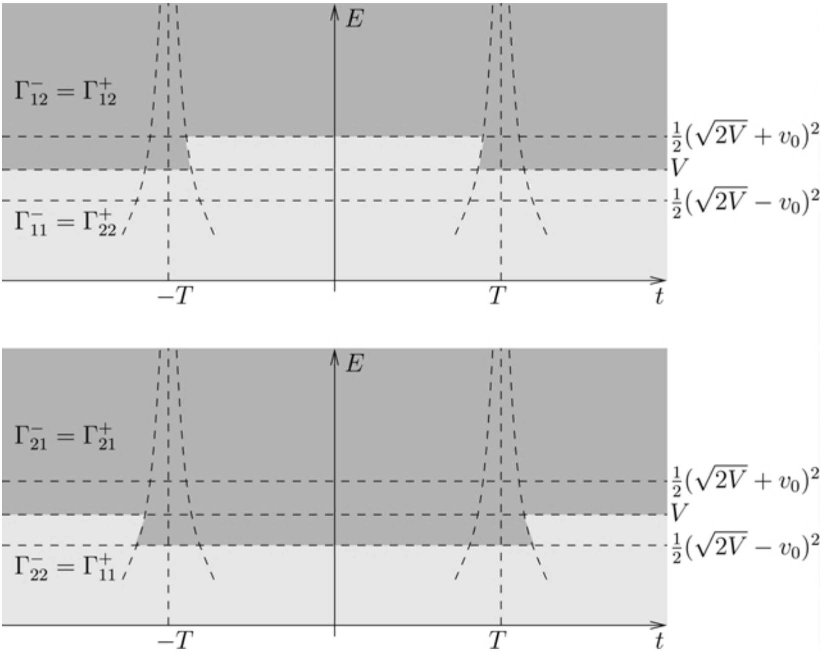

Fig. 10. Portions of phase space corresponding to transmitted (dark shaded) and reflected (light shaded) trajectories with labels +/− corresponding to outgoing/incoming data. The curves on the right halves correspond to $t = T \pm \frac{v_0}{\sqrt{2E}} T$.

- $\Gamma^-_{21} = \Gamma^+_{21}$. In this case the slope of free trajectories is $v = -\sqrt{2E} < 0$. As a result the critical energy E_c is

$$E_c = V \qquad \text{if} \quad |t| > T + \frac{v_0}{\sqrt{2E}} T,$$

$$E_c = \frac{1}{2}(\sqrt{2V} - v_0)^2 \qquad \text{if} \quad |t| \leqslant T + \frac{v_0}{\sqrt{2E}} T.$$

This portion of phase space is drawn dark shaded in the lower part of Fig. 10.

5.5. Classical Scattering from a Battery

This example shows that, in the classical case, static scattering data *cannot* determine the energy shift. Consider the classical version of the battery, see Section 2.2, with Hamiltonian function $h(x, p) = (p - A)^2/2$

and gauge $A(x,t) = t\phi'(x)$ of compact support. Clearly, this describes particles which get accelerated as they cross the pump, whence there is an energy shift. More formally, the quantity $f(x,p) = (p-A)^2/2 + \phi$ is a constant of motion, as it is verified from Newton's equation $(d/dt)(p-A) = -\dot{A} = -\phi'$. In the leads, $f = p^2/2 + \phi$, which implies that the energy $E = p^2/2$, as defined there, gets shifted by $\mathscr{E} = -\phi|_{-\infty}^{\infty}$ if a particle crosses the battery from left to right. On the other hand, for each static scatterer, $p-A$ is a constant of motion, whence the static scattering maps all equal the identity map! The quantum mechanical phase information, which was present in the static S-matrix and determined the energy shift, is of course unavailable here.

6. GEOMETRY AND TOPOLOGY

When a pump undergoes a complete cycle, so does the scattering matrix $S(E,t)$. The rows of the matrix define unit vectors in $\mathbf{C}^n$ and the charge transport in the jth channel can be interpreted in terms of geometric properties of these vectors.

As we shall explain in Section 6.2, the charge transport in the jth lead is the integral of the "global angular form" along the path of the jth row of the S-matrix during a cycle. *This integral need not yield an integer multiple of* 2π. Computing this angle is formally the same as computing Berry's phase.[10] That this phase has direct physical significance is related to the fact that a quantum pump is a wave pump. As with all problems in parallel transport, the charge transport *in a closed cycle* can also be computed by integrating a "curvature" over a surface spanning this cycle.

6.1. Charge Transport and Berry's Phase

Let

$$|\psi_j\rangle = \begin{pmatrix} S_{j1} \\ S_{j2} \\ \vdots \\ S_{jn} \end{pmatrix} \in \mathbf{C}^n \tag{6.1}$$

be the transpose of the jth row of the frozen S matrix, evaluated at the Fermi energy. Yet another rewriting of the BPT formula at zero temperature is as

$$2\pi\langle dQ\rangle_j = i\langle\psi_j \,|\, d\psi_j\rangle. \tag{6.2}$$

The expression on the right hand side is familiar from the context of adiabatic connections and Berry's phase.[10] To simplify notation we shall fix a row, say the first, and drop the index j.

There is an important conceptual difference between Berry's phase associated to a quantum state $|\psi\rangle$ and the phases that arise in the study of a row of the S-matrix $|\psi\rangle$. In the usual Berry's phase setting one starts with a circle of Hamiltonians to which one associates a (unique) circle of *projections* $|\psi\rangle\langle\psi|$, say on the ground state. To represent these projections in terms of a circle of eigenvectors $|\psi\rangle$ one needs to choose a reference phase arbitrarily for each point on the circle. The physical evolution picks its own phase via the Schrödinger equation, which is known to give parallel transport in the adiabatic limit.[15] Berry's connection is given by a formula similar to the right hand side of Eq. (6.2), and measures the accumulated difference between the physical phase (determined by parallel transport) and the reference phase. At the end of a closed cycle, the reference phase returns to its original value, so the accumulated difference is exactly the change in phase of the physical wavefunction.

A cycle of a pump, by contrast, generates a path of vectors $|\psi\rangle$ of the scattering matrix, not a path of projections. No choice of a phase needs to be made, as the phases are all fixed by solving the scattering problem. In particular, the vector $|\psi\rangle$ always returns to itself after a complete cycle of the pump. However, one can still ask how the accumulated phase (namely zero) compares to that determined by parallel transport, and Berry's connection still measures the difference. Only the interpretation is different. Rather than measuring the extent to which (physical) parallel transport fails to close on itself, in this context the integral of Berry's connection measures the extent to which (physical) closed evolution fails to be parallel.

6.2. Global Angular Form

In differential geometry, the deviation from parallel transport can be described intrinsically, without reference vectors, by using the *global angular form*, which we now describe.

If the projection $|\psi\rangle\langle\psi|$ is fixed,

$$|\psi\rangle = e^{i\gamma}\,|\psi_0\rangle, \tag{6.3}$$

then the accumulated angle is obvious: the change in angle is $\int d\gamma = \int -i\langle\psi\,|\,d\psi\rangle$.

[15] By choosing the energy of the state to be zero one can always get rid of the dynamic phase.

Now, how do we compare angles of vectors when the projections are not fixed? To do this, we need a rule for taking one vector to another without changing its global phase. A natural way to do so is to impose that there be no motion in the "direction" $|\psi\rangle\langle\psi|$. Explicitly, we say that $|\psi\rangle$ is parallel transported if

$$|\psi\rangle\langle\psi \mid d\psi\rangle = 0. \tag{6.4}$$

For parallel transport, $-i\langle\psi \mid d\psi\rangle$ is of course zero.

If we imagine an arbitrary path as a combination of parallel transport and additional angular change, then

$$-i\langle\psi \mid d\psi\rangle \tag{6.5}$$

precisely measures the component of motion in the "change the angle" direction. Since this expression is defined globally, without need of reference vectors, it is called the global angular form.

We can now compute the phase difference accumulated along any path connecting two vectors. The path may be either open or closed, and the integral of the global angular form makes sense in either case. The geometric content of the BPT formula is that expected charge transport is $-1/2\pi$ times the integral of the global angular form along the path.

6.3. Curvature

In the previous section we identified charge transport with the integral of the global angular form (6.5) along a path. Remarkably, when the path is closed, one can compute the total charge transport without knowing the phase of $|\psi_j\rangle$, relying only on the projection $|\psi_j\rangle\langle\psi_j|$. For a closed cycle one can relate the line integral on the boundary of a disk ∂D to a surface integral on the disk D via Stokes

$$2\pi\langle Q\rangle_j = i\int_{\partial D}\langle\psi_j \mid d\psi_j\rangle = i\int_D\langle d\psi_j \mid d\psi_j\rangle. \tag{6.6}$$

In the context of pumps this identity is known as Brouwer's formula.[11]

Remark 6.1. For other ways to rewrite Eq. (6.6), use the identities

$$i\langle d\psi_j \mid d\psi_j\rangle = -i(dS\wedge dS^*)_{jj} = -i\,\mathrm{Tr}\,\hat{P}_j(d\hat{P}_j\wedge d\hat{P}_j)\,\hat{P}_j, \tag{6.7}$$

where $\hat{P}_j = S^*P_jS$ is the projection onto the state feeding channel j. The r.h.s. is the trace of the curvature of the connection $\hat{P}_j d$ (see, e.g., ref. 5, Section 9.5).

We shall now describe a different interpretation of Brouwer's formula that focuses on the Wigner time delay and the energy shift. We consider the charge transport in a cycle, so t is an angle. By Eq. (A.26), and assuming no semi-bound states, so $\mathscr{E}(0, t) = 0$, the charge transport in a cycle is

$$2\pi \langle Q \rangle_j = \int_C dE \wedge dt \; \Omega_{jj} \tag{6.8}$$

where C is the cylinder $[0, \mu] \times S$. Now

$$\Omega_{jj} \, dE \wedge dt = d\mathscr{E}_{jj} \wedge dt + dE \wedge d\mathscr{T}_{jj} = -i(dS \wedge dS^*)_{jj}. \tag{6.9}$$

The difference between this formula and Eq. (6.6) is the domain of integration: A disc in Brouwer's formula, and a cylinder here. However, since $\mathscr{E}(0, t) = 0$ the bottom of the cylinder may be pinched to a point and the cylinder turns to a disk. The r.h.s. is the trace of the curvature of the connection $\hat{P}_j d$ (see, e.g., ref. 5, Section 9.5) or of its connection 1-form $i[(dS)\, S^*]_{jj} = \mathscr{E}_{jj}\, dt - \mathscr{T}_{jj}\, dE$. Similar equations are found in the context of the quantum Hall effect[35] (see, e.g., ref. 5, Section 11.3), but, unlike there, $\int_{E_-}^{\mu} \oint dE \wedge dt \; \Omega(E, t)_{jj}$ is not a Chern number as a rule, since the integration manifold has a boundary.

6.4. The Two Channel Case

The two channel case is particularly simple. $|\psi\rangle = \binom{\mathrm{r}}{\mathrm{t}'}$ lives in S^3. The projection associated to $|\psi\rangle$ can be identified with a point on S^2 according to

$$|\psi\rangle\langle\psi| = \frac{1 + \hat{n} \cdot \vec{\sigma}}{2} \tag{6.10}$$

where $\hat{n}$ is a unit vector in $\mathbf{R}^3$ and $\vec{\sigma}$ is the triplet of Pauli matrices. Equation (6.6) then says that the charge transport is half the spherical angle.

The claim that one can compute the charge transport in a closed cycle while forfeiting all knowledge of the global phase means, in the 2-channel case, that all that matters is $z = \mathrm{r}/\mathrm{t}'$. z lives in $\mathbf{CP}^1 = \mathbf{C} \cup \{\infty\}$ and is related to $\hat{n}$ above by stereographic projection

$$|\psi\rangle \to (2\,\mathrm{Re}(\mathrm{r}\bar{\mathrm{t}}'), 2\,\mathrm{Im}(\mathrm{r}\bar{\mathrm{t}}'), |\mathrm{r}|^2 - |\mathrm{t}'|^2) = \left(\frac{2\,\mathrm{Re}(z)}{1+|z|^2}, \frac{2\,\mathrm{Im}(z)}{1+|z|^2}, \frac{|z|^2 - 1}{1+|z|^2} \right). \tag{6.11}$$

The curvature

$$i(d\bar{\mathrm{r}}\, d\mathrm{r} + d\bar{\mathrm{t}}'\, d\mathrm{t}') = i(1+|z|^2)^{-2}\, d\bar{z}\, dz, \tag{6.12}$$

can be written entirely in terms of z. The current pumped by a small loop in parameter space can therefore be computed by a calculation on S^2.

For large loops, however, things are more subtle. If a path in parameter space maps to the equator, is the bounding region the northern hemisphere (area $+2\pi$) or the southern hemisphere (signed area -2π)? Because of this ambiguity, the path in S^2 only determines the fractional part of the expected charge transported, not the integral part. In particular, if the path on the unit sphere is trivial—the ratio $z = \mathrm{r}/\mathrm{t}'$ is constant—then the fractional part is zero and the charge transported is an integer. The bicycle pump, where t' is identically zero, is an example of this quantized transport.

How, then, can one determine also the integral part without a knowledge of the global phase? Consider a region in parameter space bounded by our path. The integral part is how many times it wraps around S^2 (i.e., the degree of the map). For the bicycle pump, this is counting (with sign and multiplicity) how many points on the unit square $[0, 1] \times [0, 1]$ correspond to a particular value of z, say $z = 0$. In fact, since we have already computed that the charge transport in each cycle is n, there must be n points in the interior of the square where the potential is *reflectionless* at the Fermi energy.

6.5. Chern and Winding Numbers

Part of the motivation for pumps is as standards of charge transport, whence quantization is an issue. In this section we want to explain why Chern numbers in quantum pumps must vanish. Instead, in some cases, winding numbers play a role.

The Hopf fibration gives the unit sphere $S^{2n-1} \subset \mathbf{C}^n$ the structure of a $U(1)$ principal bundle over $\mathbf{CP}^{n-1}$ via the map

$$\pi\colon S^{2n-1} \longrightarrow \mathbf{CP}^{n-1} \tag{6.13}$$

$$|\psi\rangle \longrightarrow |\psi\rangle\langle\psi|, \tag{6.14}$$

where we realize $\mathbf{CP}^{n-1}$ as the set of all rank-1 projections in $\mathbf{C}^n$.

Chern numbers in transport theory[38] typically arise as follows. The physical parameter space is a closed surface, $\mathscr{M}$, say a sphere or a torus. The Hamiltonian, acting on the vector space $\mathbf{C}^n$, is then a function on $\mathscr{M}$, and any one of its simple eigenvalues map $\mathscr{M}$ to $\mathbf{CP}^{n-1}$. The pullback of the Hopf fibration is then a $U(1)$ bundle over parameter space, with local geometry and possibly nontrivial topology. The integrated curvature is a Chern number, and may be nonzero.

In adiabatic pumps, however, the frozen S matrix defines a map from $\mathscr{M}$ directly to S^{2n-1}, and indirectly to $\mathbf{CP}^{n-1}$. This gives a trivialization of the bundle, and shows that all Chern numbers are zero. Besides, as seen from Eq. (6.6), charge transport is the integral of the Chern character $i\langle d\psi_j \mid d\psi_j\rangle$ over a surface D with boundary, and thus not given by a Chern number.

Despite the nonexistence of Chern numbers, quantization may occur in some examples. If a pump fixes the projection $|\psi\rangle\langle\psi|$, as in (6.3), then $\oint \langle dQ\rangle$ is the winding number of $e^{i\gamma}$.[3, 7] Alternatively, the curvature Eq. (6.7) can be computed in terms of $\hat{P}_j = \pi(|\psi\rangle)$, cf. Eq. (6.12), and the integral (6.6) thus performed over $\pi(D)$. The condition (6.3) means $\partial\pi(D) = \varnothing$, which again shows that $\oint \langle dQ\rangle$ is an integer.

An example where this quantization occurs is the U-turn pump, Section 5.2: The charge transport in a cycle is the winding number of the map from the circle of fluxes to the circle of complex numbers of modulus one. A small change of the parameters underlying Fig. 8 will only modify $k_F\ell$ in the effective description by Eq. (5.2) and thus preserve quantization. On the other hand, if the U-turn pump is viewed as an example of a Schrödinger operator on a graph, then a generic perturbation in this class will destroy quantization.

6.6. Geometry of Dissipation and Noise

Equations (1.6) and (1.9) that describe dissipation and entropy (and hence also noise) currents have a simple geometric interpretation in terms of the fiber bundle $S^{2n-1} \to \mathbf{CP}^{n-1}$. The jth row of $\mathscr{E}$ describes the velocity of $|\psi\rangle$ in S^{2n-1}. Of this, $\mathscr{E}_{jj}$ is the projection of this velocity onto the fiber, and $\mathscr{E}_{jk}$, with $k \neq j$, give the projection of this velocity onto $\mathbf{CP}^{n-1}$. The current $\langle \dot{Q}_j\rangle$, and the minimal dissipation $|\mathscr{E}_{jj}|^2/4\pi$, are both functions of motion in the fiber, while the excess dissipation

$$\langle \dot{E}_j\rangle - \mu\langle \dot{Q}_j\rangle - \pi\langle \dot{Q}_j\rangle^2 = \frac{1}{4\pi} \sum_{k\neq j} |\mathscr{E}_{jk}|^2 \tag{6.15}$$

is the "energy" (that is, squared velocity) associated with motion in the base. In particular, a pump operation is of the form (6.3) if and only if the bound Eq. (4.18) is saturated, or equivalently if the noise at $T > 0$ or at $T = 0$ vanishes, see Eqs. (1.9) and (B.19). Such pumps may be called *optimal*[7] w.r.t. the jth channel.

In an interesting piece of work, Mirlin and Makhlin[26] relate the problem of finding a cycle with minimal noise production at $T = 0$ to the problem of finding a minimal surfaces supported by a given loop. This result is outside the scope of transport properties which are local in time, as it deals with $T = 0$ and the noise associated with a complete cycle.

APPENDIX A. ALTERNATIVE PERSPECTIVES ON BPT

In this appendix we analyze the BPT formula from several different perspectives that shed light on its physical and mathematical content and on the semiclassical interpretation of the matrix of energy shift.

A.1. An Axiomatic Derivation of BPT

The pedestrian argument of Section 2 does not extend beyond the two channel case. This is because with more than two channels, a general variation dS cannot be described in terms of known physical processes. One can, nevertheless, derive BPT from general and simple physical considerations, without recourse to formal perturbation expansions in scattering theory. The BPT formula follows from the following natural axioms:

1. Existence and Bilinearity: There exist universal (complex) coefficients a^m_{ijkl} such that

$$dQ_m = \sum_{ijkl} a^m_{ijkl}\, dS_{ij}\, \bar{S}_{kl} + \text{complex conjugate}. \tag{A.1}$$

2. Covariance: The formula is covariant under permutation of the channels. In particular, it is invariant under permutations of the channels other than the mth.

3. Gauge invariance: The formula is unchanged by time-independent gauge transformations, and also under time-independent changes in the fiducial points.

4. Cluster: If the system consists of two subsystems, disconnected from one another, then the currents in each subsystem depend only on the part of the S matrix that governs that subsystem.

5. Landauer: If a voltage, applied to a single lead $m' \neq m$, is modeled by a time-dependent gauge transformation, then dQ_m is given by the Landauer formula where the transmission probability is given by the scattering probability $m' \to m$.

6. Birman–Krein[39] or Friedel[19] sum rule:

$$\sum_j dQ_j = \frac{i}{2\pi} d\log(\det S) = \frac{i}{2\pi} \mathrm{Tr}(dS\, S^\dagger).$$

The physical motivations for most of the axioms are clear. For example, bilinearity comes from the fact that the current is an interference effect between the original outgoing wavefunction (described by S) and an additional piece (described by dS). The one axiom that seems the most arbitrary is existence—the assumption that charge transport at $T=0$ is determined by the scattering matrix at the same time and at the Fermi energy alone.

By covariance, it suffices to study the current on the first channel, dQ_1 (and drop the superindex in a). Henceforth, Latin indices will run from 1 to n, while Greek indices will run from 2 to n.

The most general bilinear (A.1) vanishing identically on unitaries S and their variations dS is of the form $a_{ijkl} = e_{jl}\delta_{ik} + d_{ik}\delta_{jl}$ with hermitian matrices (e_{jl}) and (d_{ik}). Indeed, by $SS^* = S^*S = 1$ the matrices $(dS)\,S^*$ and $(dS)^*\,S$ are anti-hermitean, which implies vanishing of the stated bilinear form. We can thus fix a_{ijkl} in (A.1) by imposing the uniqueness constraints that $\sum_\alpha a_{\alpha j\alpha l}$ and $\sum_\alpha a_{i\alpha k\alpha}$ are anti–hermitian.

We shall now see that by axiom 3

$$a_{ijkl} = c_{ij}\delta_{ik}\delta_{jl}. \tag{A.2}$$

Indeed, if we move the fiducial point on the ith channel by distance ξ_i, the S-matrix transforms by

$$S_{ij} \to S_{ij} e^{ik_{\mathrm{F}}(\xi_i+\xi_j)}, \tag{A.3}$$

and so $a_{ijkl} \to a_{ijkl} e^{ik_{\mathrm{F}}(\xi_i+\xi_j-\xi_k-\xi_l)}$. The only invariant terms are those with $i=k$ and $j=l$ or with $i=l$ and $j=k$. Similarly, gauge transformations send

$$S_{ij} \to S_{ij} e^{i(\phi_i-\phi_j)}. \tag{A.4}$$

Now the invariant a_{ijkl} terms are those with $i=k$ and $j=l$ or with $i=j$ and $k=l$. Putting the two selection rules together gives Eq. (A.2). At this point Eq. (A.1) reduces to

$$dQ_1 = \sum_{ij} c_{ij}\, dS_{ij}\, \bar{S}_{ij} + \text{complex conjugate}, \tag{A.5}$$

with the constraint that the coefficients c_{ij} are pure imaginary.

By the cluster property $c_{\alpha\beta}$ must all vanish, for otherwise dQ_1 will be affected also by channels disconnected from it. Now $c_{1\alpha}$ and $c_{\alpha 1}$ are independent of α by permutation symmetry. We can therefore write Eq. (A.1) as

$$dQ_1 = c_1\, dS_{11}\, \bar{S}_{11} + c_2 \sum_k dS_{1k}\, \bar{S}_{1k} + c_3 \sum_k dS_{k1}\, \bar{S}_{k1} + \text{complex conjugate}, \tag{A.6}$$

where $c_1 = c_{11}$, $c_2 = c_{1\alpha}$, and $c_3 = c_{\alpha_1}$. Summing dQ_j over all channels, using that c_1, c_2, c_3 are pure imaginary, and setting the result to agree with the Birman–Krein formula gives

$$\sum_j dQ_j = 2ic_1\, \mathrm{Im} \sum_j dS_{jj}\, \bar{S}_{jj} + 2(c_2 + c_3)\, \mathrm{Tr}(dS\, S^\dagger) = \frac{i}{2\pi}\, \mathrm{Tr}(dS\, S^\dagger). \tag{A.7}$$

Thus $c_1 = 0$ and $4\pi(c_2 + c_3) = i$.

What remains is to distinguish between c_2 and c_3. Imagine modeling a voltage V on channel α by a time dependent vector potential that shifts the phase of the wavefunction on the αth channel by $d\phi$. Equating with Landauer gives

$$dQ_1 = -2i(c_2\, |S_{1\alpha}|^2 - c_3\, |S_{\alpha 1}|^2)\, d\phi = \frac{1}{2\pi}\, |S_{1\alpha}|^2\, d\phi. \tag{A.8}$$

Since (for $n \geqslant 3$) $|S_{\alpha 1}|^2$ and $|S_{1\alpha}|^2$ are independent, this implies that $c_2 = i/4\pi$ and $c_3 = 0$. We thus obtain BPT for $n \geqslant 3$.[16]

A.2. Classical Pumps

We next examine classical pumps and the roles of the classical time delay and energy shift. Although there are important differences in detail, the relation between energy shift and expected current in the classical case is qualitatively similar to the BPT formula for the quantum case. By contrast, the energy shift can not be expressed in terms of static scattering data.

We picture each channel as a real half-line $x > 0$, see, e.g., Fig. 1. The classical phase space associated to a given channel is the half-plane $\{x, p \mid x > 0, p \in \mathbf{R}\}$. We can choose coordinates so that points in phase space are labelled by the pair (E, t), where E is the energy of the (classical)

[16] To get the $n = 2$ case, consider a 2-channel scatterer as a degenerate 3-channel scatterer, where the third channel is disconnected from the first two. Then S_{31} is identically zero, and the 3-channel BPT formula for dQ_1 reduces to the 2-channel formula.

particle and t its time of passage at the origin. For concreteness, let us assume a dispersion relation $\epsilon(p) = \epsilon(-p)$ with $\epsilon(p)$ increasing from 0 to ∞ as p ranges over the same interval, e.g., a quadratic dispersion. Then

$$E = \epsilon(p), \qquad t = -x/v, \qquad (v = \epsilon') \tag{A.9}$$

is a canonical transformation to the energy-time half plane $\{E, t \mid E > 0, t \in \mathbf{R}\}$, since $dE \wedge dt = dx \wedge dp$. The mapping is singular when $v = 0$. States with $t > 0$ are incoming (at time 0), while those with $t < 0$ are outgoing (at time 0). (All states are, of course, incoming in the distant past and outgoing in the distant future.)

The phase space of n disconnected channels is $\Gamma = \bigcup_{i=1}^{n} \Gamma_i = \{(E, t, i) \mid E > 0, t \in \mathbf{R}, i = 1,..., n\}$. When analyzing pumps, i.e., channels communicating through some pump proper, Γ still serves as phase space of the *scattering states*. More precisely, (E, t, i) shall be the label of the scattering state whose past asymptote is the free trajectory with these initial data. Similarly, we may indicate a scattering state by its future oriented data (E', t', j). In this way we avoid introducing the full phase space for the connected pump. However, some of these trajectories may admit only one of the two labels, as they are free for, say, $t \to -\infty$ but trapped as $t \to +\infty$. With this exception made, the relation defines a bijective map, the (dynamical) *scattering map*:

$$S: \Gamma^- \to \Gamma^+, \qquad (E, t, i) \mapsto (E', t', j), \tag{A.10}$$

where $\Gamma \setminus \Gamma^-$ are the incoming labeled trajectories which are trapped in the future, and correspondingly for $\Gamma \setminus \Gamma^+$. If (A.10) is viewed as a function of (E, t) with i fixed, the channel j is piecewise constant and the map to (E', t') symplectic. We shall illustrate S by an example in Section 5.4. The inverse map may be written as

$$S^{-1}: (E', t', j) \mapsto (E, t, i) = (E' - \mathscr{E}_d(E', t', j), t' - \mathscr{T}_d(E', t', j), i), \tag{A.11}$$

which *defines* the classical energy shift $\mathscr{E}_d$ and the time delay $\mathscr{T}_d$ as functions of the outgoing data. We remark that, for a static pump, $\mathscr{E} = 0$ and $\mathscr{T}$ is independent of t'. For adiabatic pumps, we have $\mathscr{E}_d(E', t', j) = O(\omega)$ and $\mathscr{T}_d(E', t', j) = \mathscr{T}(E', t', j) + O(\omega)$, where $\mathscr{T}$ is the time delay of the static scatterer in effect at the time of passage t', on which it then depends parametrically. Since S^{-1} preserves volume (by Liouville's theorem) and the derivative with respect to time brings in a factor of ω, we have

$$\mathscr{E}' + \dot{\mathscr{T}} = 0, \tag{A.12}$$

where $\mathscr{E}$ is the part of $\mathscr{E}_d$ of order ω^1. This relation shows that the static scattering data determine $\mathscr{E}(E', t', j)$ up to an additive function of t' and j. This is in sharp contrast to the quantum case, where $\mathscr{E}$ is fully determined by the frozen scattering matrix, see Eq. (1.2). We will further comment on the origin of this ambiguity in the classical case in Sections 3.1 and 5.5 and relate it to the lack of phase information in classical scattering.

As in the quantum case, Eq. (1.5) is the correct expression for the current in terms of the energy shift:

$$\dot{Q}_j(t) = -\int_0^\infty dE\, g'(E)\, \mathscr{E}(E, t, j), \tag{A.13}$$

where $g(E)$ is the phase space particle density in the incoming flow. We remark that in a semiclassical context g is related to the occupation density ρ by $g(E) = \rho(E)/2\pi$.

In fact, the net outgoing charge transmitted in the time interval $[0, T]$ through channel j is

$$Q_j = \int_{\Gamma_j} dE'\, dt'\, \chi_{[0,T]}(t')\, g(E) - \int_{\Gamma_j} dE\, dt\, \chi_{[0,T]}(t)\, g(E), \tag{A.14}$$

where E in the first integral is given through the map (A.11) if $(E', t', j) \in \Gamma^+$; if $(E', t', j) \in \Gamma \setminus \Gamma^+$, which may occur if E' is close to threshold energy 0 and $E < 0$, we assume that $g(E) = g(0)$, i.e., that the occupation of the bound states and threshold energies are equal.

Equation (1.5) is obtained immediately by expanding $g(E) = g(E') - g'(E')\, \mathscr{E}(E', t', j) + O(\omega^2)$ in the first integral (A.14). The contribution of the first term cancels against the second integral.

Another derivation, which is more involved, is of some interest especially in view of the semiclassical discussion of pumps in Appendix A.3. The first integral (A.14) equals

$$\int_{\Gamma_j} dE'\, dt'\, \chi_{[0,T]}(t)\, g(E) - \int_0^\infty dE' g(E)\, \mathscr{T}(E', t', j)\Big|_{t=0}^{t=T}. \tag{A.15}$$

In the adiabatic regime we may describe Γ_j, to lowest approximation, as $\Gamma_j = \bigcup_{i=1}^n \Gamma_{ij}$, where Γ_{ij} consists of states (E', t', j) originating from lead i under static scattering. W.r.t. them and to next approximation, their pre-images (E, t, i) appearing as arguments in the first integral (A.15), are displaced by the vector field $-(\mathscr{E}(E', t', j), \mathscr{T}(E', t', j))$, which is typically discontinuous across the boundaries of the Γ_{ij}'s, but divergence free otherwise by (A.12). (For an illustration, see Example 5.4 and Fig. 10 there.) As a result, that integral differs from the second integral (A.14) by

$$-\sum_{i=1}^{n}\int_{\partial\Gamma_{ij}}(d\sigma_E\,\mathscr{E}(E',t',j)+d\sigma_t\,\mathscr{T}(E',t',j))\,\chi_{[0,T]}(t)\,g(E), \qquad \text{(A.16)}$$

where $(d\sigma_E, d\sigma_t)$ is the outward normal to $\partial\Gamma_{ij}$. Within $\bigcup_{i=1}^{n}\partial\Gamma_{ij}$ we may distinguish between boundary parts contained in the boundary $\{E=0\}$ of Γ_j, and inner boundaries. The contribution of the former is $\int_0^T dt\,g(0)\,\mathscr{E}(0,t,j)$ and, mostly for comparison with the promised semiclassical derivation, we formally write that of the latter as $\int_{\Gamma_j}\Omega(E,t,j)\,\chi_{[0,T]}(t)\,g(E)$, where $\Omega(E,t,j)$ is a distribution supported on the inner boundaries. Since the map (A.10) is bijective on Γ except for bound states, the displacements of the sets Γ_{ij} are such that $\sum_{j=1}^{n}\Omega(E,t,j)=0$. In summary, we obtain

$$Q_j=\int_0^T dt\,g(0)\,\mathscr{E}(0,t,j)-\int_0^\infty dE\,g(E)\,\mathscr{T}(E,t,j)\Big|_{t=0}^{t=T}$$
$$+\int_0^\infty dE\int_0^T dt\,g(E)\,\Omega(E,t,j) \qquad \text{(A.17)}$$

and, by differentiating w.r.t. T,

$$\dot{Q}_j=g(0)\,\mathscr{E}(0,t,j)-\int_0^\infty dE\,g(E)\,\dot{\mathscr{T}}(E,t,j)+\int_0^\infty dE\,g(E)\,\Omega(E,t,j). \qquad \text{(A.18)}$$

The first term on the r.h.s. describes the release and trapping from bound states. The middle term describes the depletion of the outgoing flow as a result of a time delay increasing over time, since effectively no charge is exiting during a time $d\mathscr{T}$. The last term describes electrons that are reshuffled between leads, but with no withholdings since $\sum_{j=1}^{n}\Omega(E,t,j)=0$.

From (A.18), Eq. (A.13) can be recovered: Let $[E_k(t),E_{k+1}(t)]$, $(k=0,1,\dots)$ be the intervals of the partition of $[0,\infty)$ on which $\mathscr{E}$, $\mathscr{T}$ are continuous, and $\Delta_k\mathscr{E}=\mathscr{E}(E_k+,t,j)-\mathscr{E}(E_k-,t,j)$, $\Delta_k\mathscr{T}=\mathscr{T}(E_k+,t,j)-\mathscr{T}(E_k-,t,j)$, $(k=1,2,\dots)$ the values of their discontinuities at the endpoints. Then

$$\int_0^\infty dE\, g(E)\, \Omega(E,t,j) = \sum_{k\geqslant 1} g(E_k)(\Delta_k \mathscr{E} - \dot{E}_k\, \Delta_k \mathscr{T}),$$

$$-\int_0^\infty dE\, g(E)\, \dot{\mathscr{T}}(E,t,j) = -\sum_{k\geqslant 0} \int_{E_k}^{E_{k+1}} dE\, g(E)\, \dot{\mathscr{T}}(E,t,j) \qquad \text{(A.19)}$$

$$+\sum_{k\geqslant 1} g(E_k)\, \dot{E}_k\, \Delta_k \mathscr{T}.$$

Using Eq. (A.12) and integration by parts, the first term on the r.h.s. of (A.19) can be written as

$$\sum_{k\geqslant 0} \int_{E_k}^{E_{k+1}} dE\, g(E)\, \mathscr{E}'(E,t,j)$$

$$= -g(0)\, \mathscr{E}(0,t,j) - \sum_{k\geqslant 1} g(E_k)\, \Delta_k \mathscr{E} - \sum_{k\geqslant 0} \int_{E_k}^{E_{k+1}} dE\, g'(E)\, \mathscr{E}(E,t,j). \qquad \text{(A.20)}$$

By collecting terms, we recover Eq. (A.13).

A.3. Currents and the $\mathscr{T}$–$\mathscr{E}$ Uncertainty

Finally, we present a semiclassical derivation of Eq. (1.5), where we however take for granted the physical meaning of the energy shift Eq. (1.2), which will be established in Section 3.1. Since the time delay is a matrix, see Eq. (1.3), we should, as a preliminary, point out that it is the diagonal element $\mathscr{T}_{jj}(E,t)$ which has the meaning of the average time delay of a particle exiting channel j. In fact, consider an incoming wave packet $\int dk\, e^{-i(kx+\epsilon(k)\,t)}\varphi(k)$ in channel i centered on the trajectory $-x = \epsilon'(k)\, t + c$. The part of it scattered into lead j is $\int dk\, e^{i(kx-\epsilon(k)\,t)} S_{ji}(\epsilon(k), t)\, \varphi(k)$ and is associated with $x = \epsilon'(k)(t - (\arg S_{ji})') + c$ (with $' = d/dE$ on $\arg S_{ji}$), which implies a time delay of $(\arg S_{ji})'$. Averaging this with the probability $|S_{ji}|^2$ for the particle to have come from channel i, we find for the average delay

$$\sum_{i=1}^{n} |S_{ji}|^2\, (\arg S_{ji})' = \operatorname{Im} \sum_{i=1}^{n} \bar{S}_{ji} S'_{ji} = \mathscr{T}_{jj}. \qquad \text{(A.21)}$$

The net outgoing charge in the time interval $[0, T]$ is at order ω

$$\langle Q\rangle_j = \frac{1}{2\pi}\int_0^\infty dE' \int_0^T dt'\, \rho(E) - \frac{1}{2\pi}\int_0^\infty dE \int_0^T dt\, \rho(E), \qquad \text{(A.22)}$$

where E in the first integral is given through the map

$$\Phi\colon (E', t') \mapsto (E, t) = (E' - \mathscr{E}_{jj}(E', t'), t' - \mathscr{T}_{jj}(E', t')), \tag{A.23}$$

which describes the effect of the pump on the energy and the time of passage of an electron in terms of the outgoing data (E', t'). This is similar to the classical Eq. (A.11) except that $\mathscr{E}$ and $\mathscr{T}$ are now defined in terms of the quantum mechanical frozen scattering matrix S, see Eqs. (1.2) and (1.3). Energies E' close to the threshold $E' = 0$ may not be in the domain of the map Φ. Similarly, energies E may there fail to be in its range. These situations correspond to electrons released from, resp. trapped into, a bound state of the pump.

The BPT formula, Eq. (1.5), is again obtained immediately by expanding $\rho(E) = \rho(E') - \rho'(E')\, \mathscr{E}_{jj}(E', t') + O(\omega^2)$ in the first integral (A.22). The contribution of the first term cancels against the second integral. A further derivation, which is longer but adds another interpretation to the result, is by using Φ as a change of variables. The Jacobian of (A.23) is $1 - \Omega_{jj}(E', t')$, where Ω_{jj} is the divergence of the displacement $(\mathscr{E}_{jj}, \mathscr{T}_{jj})$. As a matrix, Ω is the time delay-energy shift uncertainty introduced in Eq. (1.4):

$$\Omega = i[\mathscr{T}, \mathscr{E}] = i(\dot{S}S^{*\prime} - S'\dot{S}^*) = \mathscr{E}' + \dot{\mathscr{T}}. \tag{A.24}$$

Since Ω is formally of order $O(\omega)$, the Jacobian is close to 1 and the map (A.23) is invertible. After changing variables to (E, t) the first integral (A.22) extends over $(E, t) \in \Phi([0, \infty) \times [0, T])$, which differs from $[0, \infty) \times [0, T]$ to leading order by displacements $-\mathscr{E}_{jj}(E, t)$ along $E = 0$ and $-\mathscr{T}_{jj}(E, t)$ along $t = 0, T$. This yields

$$\begin{aligned} 2\pi\langle Q\rangle_j = {} & -\int_0^T dt\, \rho(E)\, \mathscr{E}_{jj}(E, t)\Big|_0^\infty - \int_0^\infty dE \rho(E)\, \mathscr{T}_{jj}(E, t)\Big|_{t=0}^{t=T} \\ & + \int_0^\infty dE \int_0^T dt\, \rho(E)\, \Omega_{jj}(E, t), \end{aligned} \tag{A.25}$$

and the differential version thereof is

$$2\pi\langle \dot{Q}\rangle_j\,(t) = \rho(0)\, \mathscr{E}_{jj}(0, t) - \int_0^\infty dE\, \rho(E)\, \dot{\mathscr{T}}_{jj}(E, t) + \int_0^\infty dE\, \rho(E)\, \Omega_{jj}(E, t). \tag{A.26}$$

Upon inserting (A.24) and performing an integration by parts on $\rho\mathscr{E}'_{jj}$, Eq. (1.5) is recovered. The interpretation of the three terms is the same as given after Eq. (A.18). For the first term, with bound states now quantized, this is further discussed in the remark below. As for the last term, notice that $\sum_{j=1}^{n} \Omega_{jj} = 0$ still holds true because of Eq. (1.4). While generally, and in contrast to the classical case, Ω may have full support in phase space, it remains true that it vanishes if scattering is deterministic: If on some open subset of phase space

$$S_{ji}(E, t) = 0 \qquad \text{for} \quad i \neq \pi(j), \tag{A.27}$$

where π is some fixed permutation of the channels, then S^* is in the same manner related to π^{-1}, and $\mathscr{E}$, $\mathscr{T}$ to the identity permutation, i.e., they are both diagonal matrices. Hence $\Omega = 0$ by (1.4).

Remark A.1. The first term on the r.h.s. of (A.26) typically consists of delta functions located at times t where the pump has a semi-bound state at a band edge, i.e., a state which can be turned either into a bound state or a scattering state by an arbitrarily small change of the pump configuration. We illustrate this for $\epsilon(k) = k^2$, and first claim: either $S(0, t) \equiv \lim_{E \downarrow 0} S(E, t) = -1$, or the (static) pump at time t admits a semi-bound state. This is seen as follows: For each $k \in \mathbf{C}$ the $2n$ plane waves

$$e_i \cos kx, \qquad e_i \frac{\sin kx}{k}, \tag{A.28}$$

($\{e_i\}_{i=1}^{n}$ being the standard basis of $\mathbf{C}^n$), form a basis of solutions with energy k^2 in the n disconnected leads. Upon connecting them to the scatterer an n-dimensional subspace of solutions is left, which depends analytically on k. Since the dependence of (A.28) is also analytic, solutions may be written as

$$\psi_k(x) = \sum_{i=1}^{n} \alpha_i e_i \cos kx + \beta_i e_i \frac{\sin kx}{k}, \tag{A.29}$$

with amplitudes $\alpha = (\alpha_1, ..., \alpha_n)$, $\beta = (\beta_1, ..., \beta_n)$ satisfying a set of linear equations

$$A(k)\, \alpha + B(k)\, \beta = 0 \tag{A.30}$$

with analytic $n \times n$ coefficient matrices A, B. As (A.30) defines an n-dimensional subspace, we have $\operatorname{rank}(A, B) = n$. For $k = 0$ (A.28) reduce to e_i, $e_i x$. By a semi-bound state we mean more precisely a bounded solution $\psi_0(x)$, i.e., one with $\beta = 0$ in (A.29). Its existence is tantamount to $\det A(0) = 0$. If $\det A(0) \neq 0$, (A.30) can be solved for α at small k:

$\alpha = -A(k)^{-1} B(k) \beta$, with arbitrary $\beta \in \mathbf{C}^n$. For $k > 0$, the scattering matrix maps the incoming part of (A.29) to its outgoing part, $ik\alpha + \beta = S(k^2)(ik\alpha - \beta)$. Thus

$$S(k^2) = (-ikA(k)^{-1} B(k) + 1)(-ikA(k)^{-1} B(k) - 1)^{-1} \to -1, \qquad (k \to 0). \tag{A.31}$$

This proves the claim, and in particular that $\mathscr{E}(0, t) = 0$ except at times t when the scatterer has a semi-bound state. To discuss its behavior there, say this happens at $t = 0$, we assume generically that $C(k, t) = B(k, t)^{-1} A(k, t)$ $(= C(k, t)^*)$ has a simple eigenvalue $\gamma(k, t)$ with a first order zero at $k = t = 0$. Let P be its eigenprojection at crossing and let $\sigma = \operatorname{sgn} \dot{\gamma}(0, 0)$ be the crossing direction. Then, we claim,

$$\lim_{E \downarrow 0} \mathscr{E}(E, t)\, dt = -2\pi\sigma P \delta(t)\, dt, \tag{A.32}$$

so that in the process, by (2.1), the charge

$$-\lim_{E \downarrow 0} \frac{1}{2\pi} \int_{-\epsilon}^{\epsilon} \operatorname{tr} \mathscr{E}(E, t)\, dt = \sigma \tag{A.33}$$

is captured at arbitrarily small energy. Since the l.h.s. also equals $\lim_{E \downarrow 0} \arg\det S(E, t)|_{-\epsilon}^{\epsilon}$, (A.33) states that the phase of $S(0, t)$ changes by 2π upon capture of a bound state, which is a dynamical version of Levinson's theorem. The proof of (A.32) rests on the approximation of (A.31)

$$S(k^2, t) = \frac{ikP - (\gamma'(0, 0)\, k + \dot{\gamma}(0, 0)\, t)}{ikP + (\gamma'(0, 0)\, k + \dot{\gamma}(0, 0)\, t)}, \tag{A.34}$$

valid near $k = t = 0$.

APPENDIX B. COMPARISON WITH THE THEORY OF FULL COUNTING STATISTICS

The formulas for the entropy and noise currents, Eq. (1.9), are singular in the limit $T \to 0$. This appears to be in conflict with the Lesovik–Levitov's formula (LL) which gives finite noise at $T = 0$ (see below). We shall verify here that, in fact, for $T \gtrsim \omega$, LL is consistent with our results. We shall start by recalling LL.

B.1. The Lesovik–Levitov Formula

Here we shall describe a version of the Lesovik–Levitov formalism[22] where LL is an identity rather than an (adiabatic) approximation.

Assume that in the distant past and distant future the Hamiltonian $H(t)$ of the pump coincides with H_0, the disconnected pump. Let Q_j be a projection on one the jth channels. Since the channel is fixed we suppress the index j below. It is important in this formulation that the channels are disconnected at the distant past and distant future and that $[Q, H_0]=0$. It is also assume that the initial state of the system is thermal state $\rho(H_0)$. The counting statistics can be described by means of the characteristic function $\chi(\lambda)=\sum_{n=-\infty}^{\infty} p_n e^{i\lambda n}$, where p_n is the probability for n charges having been transferred to channel j in the course of whole process. The formula is

$$\chi(\lambda)=\det(1+\rho(e^{-i\lambda Q/2}\, e^{i\lambda\hat{Q}}\, e^{-i\lambda Q/2}-1)), \qquad \hat{Q}=S_d^* Q S_d, \quad \rho=\rho(H_0) \tag{B.1}$$

where, as before, ρ is the Fermi function and $\hat{Q}$ is a projection on the states feeding the channel in question.

Remark B.1. The reason Q plays a special role is traced to the fact that the second quantized $d\Gamma(Q)$ is the number (charge) operator in the channel.

Since Q is a projection $e^{i\lambda Q}=1+(e^{i\lambda}-1)\,Q$. Using this one finds

$$\begin{aligned} e^{-i\lambda Q/2}\, e^{i\lambda\hat{Q}}\, e^{-i\lambda Q/2}-1 &= iA\sin\lambda-(1-\cos\lambda)\,A^2 \\ &\quad +2i\sin(\lambda/2)(1-\cos(\lambda/2))(Q\hat{Q}Q_\perp+Q_\perp\hat{Q}Q) \end{aligned} \tag{B.2}$$

where

$$A=\hat{Q}-Q \tag{B.3}$$

is a difference of projections. To second order in λ

$$\begin{aligned} \log\chi(\lambda) &= \operatorname{Tr}\log\left(1+i\lambda\rho A-\frac{\lambda^2}{2}\rho A^2\right)+O(\lambda^3) \\ &= i\lambda\operatorname{Tr}(\rho A)-\frac{\lambda^2}{2}\operatorname{Tr}(\rho A(1-\rho)\,A)+O(\lambda^3). \end{aligned} \tag{B.4}$$

In the last step we used the fact that Q commutes with H_0 and the cyclicity of the trace.

B.2. Charge Transport

The expectation value of charge transport into the jth channel is the first moment:

$$\langle Q \rangle_j = -i(\log \chi)'(0) = \mathrm{Tr}(\rho A) = \mathrm{Tr}((\rho(H_0 - \mathscr{E}_d) - \rho(H_0))\, Q_j). \tag{B.5}$$

This is clearly the correct result, independent of the adiabatic limit, for the rhs is precisely what one means by the change in the total charge in the jth reservoir. In the adiabatic limit $\mathscr{E}_d$ is small and hence

$$\langle Q \rangle_j \approx -\mathrm{Tr}(\rho'(H_0)\, \mathscr{E}_d Q_j) = -\frac{1}{2\pi} \int dt\, dE\, \rho'(E)\, \mathscr{E}_{jj}(E, t) \tag{B.6}$$

in agreement with BPT. In the last step we used Eq. (3.15) and Eq. (4.3).

B.3. Splitting the Noise

Noise is the variance of the distribution associated to $\chi(\lambda)$ or, more precisely, the variance per unit time. It splits into two positive terms. One term is proportional to the temperature—this is the Johnson–Nyquist noise. The second term involve correlations at different times and survives at $T = 0$. This is the quantum shot noise.

The variance is

$$\langle (\Delta Q)^2 \rangle = -(\log \chi)''|_{\lambda=0} = \mathrm{Tr}(\rho A(1-\rho)\, A). \tag{B.7}$$

Now, write

$$\rho A(1-\rho)\, A = \rho A^2(1-\rho) + \rho A[A, \rho] = \rho(1-\rho)\, A^2 + \rho[\rho, A]\, A. \tag{B.8}$$

Using the cyclicly of the trace and the average of the two terms in Eq. (B.8), we find

$$\mathrm{Tr}(\rho A(1-\rho)\, A) = \mathrm{Tr}(\rho(1-\rho)\, A^2) + \tfrac{1}{2}\, \mathrm{Tr}([\rho, A][A, \rho]). \tag{B.9}$$

Each term is positive. The Johnson–Nyquist noise is the first term

$$Q_{JN}^2 = \mathrm{Tr}(\rho(1-\rho)\, A^2) = -T\, \mathrm{Tr}(\rho' A^2) \geqslant 0, \tag{B.10}$$

and the quantum shot noise is the second term:

$$Q_{QS}^2 = \tfrac{1}{2}\,\mathrm{Tr}([\rho, \hat{Q}][\hat{Q}, \rho]) = \tfrac{1}{2}\,\mathrm{Tr}([\delta\rho, Q][Q, \delta\rho]) \geqslant 0. \tag{B.11}$$

(We have repeatedly used $[Q, H_0] = 0$.) Since the semi-classical limit of a commutator is of order $\hbar$, the quantum shot noise vanishes in the classical limit.

B.4. Thermal Noise

ρ' is a multiplication operator in E which, at low temperatures, is concentrated near μ. The symbol of A_j is:

$$A_j \Leftrightarrow a(E, t) = S^*(E, t)\, P_j S(E, t) - P_j, \tag{B.12}$$

where P_j is an $n \times n$ matrix that projects on the jth channel. The Johnson–Nyquist noise at low temperatures can be written as

$$\begin{aligned} 2\pi\, Q_{JN}^2 &= T \int_{\mathbf{R}} dt\ \mathrm{tr}(a^2(\mu, t)) = T \int_{\mathbf{R}} dt\ \mathrm{tr}(\hat{P}(t) + P - \hat{P}(t)\, P - P\hat{P}(t)) \\ &= 2T \sum_{k \neq j} \int_{\mathbf{R}} dt\ |S|_{jk}^2\ (\mu, t), \end{aligned} \tag{B.13}$$

where tr denotes a trace of $n \times n$ matrices, and we have used the fact that P and $\hat{P}$ are one dimensional projections. We see that the Johnson–Nyquist noise is proportional to the temperature and the time integral of the conductance at the Fermi energy. It is finite since for large times $H(t)$ coincides with H_0 and the scattering matrix reduces to the identity.

B.5. Shot Noise at Finite Temperatures

The symbol associated to $[\delta\rho, Q]$ is, to leading order, the matrix

$$-\rho'(E)[\mathscr{E}(E, t), P_j]$$

where, as before, P_j is the projection on the jth channel. At finite temperatures $\rho'(E)$ is a smooth function and it makes sense to look at the square of the symbol as we must by Eq. (B.11). Now

$$\mathrm{tr}[\mathscr{E}(E, t), P_j][P_j, \mathscr{E}(E, t)] = 2((\mathscr{E}^2)_{jj} - (\mathscr{E}_{jj})^2)(E, t) = 2\Delta\mathscr{E}_{jj}^2(E, t). \tag{B.14}$$

Substituting in Eq. (3.14) and using the fact that ρ' is localized near the Fermi energy, we find

$$\begin{aligned} Q_{QS}^2 &= \frac{1}{2\pi} \int dE\, dt\, (\rho'(E))^2\, \Delta\mathscr{E}_{jj}^2(E, t) \\ &= \frac{\beta}{2\pi} \int dt \int_0^1 d\rho\, \rho(1-\rho)\, \Delta\mathscr{E}_{jj}^2(\mu, t) \\ &= \frac{\beta}{12\pi} \int dt\, \Delta\mathscr{E}_{jj}^2(\mu, t) \end{aligned} \tag{B.15}$$

in agreement with Eq. (1.9).

B.6. Shot Noise at $T=0$

The result at finite temperature may suggest that the noise over a pump cycle diverges as $T \to 0$. This is not the case. At $T=0$ the symbol ρ' is a distribution and it is not permissible to multiply them as we did in Eq. (B.15). However, the problem can be easily avoided by simply not using the r.h.s. of Eq. (B.11) but instead the middle identity. As before, we approximate the symbol of $\hat{Q}$ by its value on the Fermi energy

$$\hat{Q}_j \Leftrightarrow S^*(E, t)\, P_j S(E, t) \approx S^*(\mu, t)\, P_j S(\mu, t) = q_j(t). \tag{B.16}$$

This approximation makes $\hat{Q}_j$ a multiplication operator in t and hence

$$Q_{QS}^2 = \int_{\mathbf{R}} \int_{\mathbf{R}} dt\, dt'\, |\tilde{\rho}(t-t')|^2\, \mathrm{tr}(q(t) - q(t'))^2, \tag{B.17}$$

where $\tilde{\rho}$ is the Fourier transform of the Fermi function. At $T=0$ the Fermi function associated with chemical potential μ is

$$\tilde{\rho}(t) = \frac{i}{2\pi(t+i0)}\, e^{-it\mu}. \tag{B.18}$$

The shot noise at $T=0$, in the limit of large μ, is given by

$$Q_{QS}^2(\mu) = \frac{1}{4\pi^2} \iint dt\, dt'\, \frac{1 - |(S(\mu, t)\, S^*(\mu, t'))_{jj}|^2}{(t-t')^2}. \tag{B.19}$$

Since S is unitary the numerator vanishes quadratically as $t-t' \to 0$. It follows that the integrand is a bounded function. However, it is supported on set of infinite area made of two strips: One along the t axis and one along the t' axis. Nevertheless, the decay properties of the denominator one easily sees that the integral is convergent. The noise in a pump cycle does not diverge as $T \to 0$.

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