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EQUIVALENCE OF TOPOLOGICAL AND SCATTERING APPROACHES TO QUANTUM PUMPING

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GREGORIO ORTELLI

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Angenommen auf Antrag von

Prof. Dr. Gian Michele Graf
Prof. Dr. Markus Büttiker

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ABSTRACT. The subject of this dissertation is the transport of charge occurring in quantum pumps. These are compact devices, acting in the mesoscopic scale, connected to several leads, and controlled by some parameter varying periodically in time. They achieve a net transport from one lead to another at each cycle of the pump.

Different theories exist which describe quantum pumping, originating from different idealizations of the devices. In the present work we will focus on two descriptions of pumping in the adiabatic regime.

In the topological approach to quantum pumping the pump is considered from a microscopic viewpoint. It is modeled by an infinitely extended potential, with a periodic time dependence. The potential has to produce a spectral gap in the instantaneous Hamiltonian, and the Fermi energy has to lie in such a gap, at all times of the cycle. The charge transported across a reference point during a cycle is found to have integer value. The reason for this quantization is of topological nature: the charge transport is identified as the Chern number of a fiber bundle. For single-channel, space periodic potentials this is a result of Thouless. We extend this result to multi-channel potentials and to non-periodic potentials.

In the scattering approach to quantum pumping the pump is considered from a macroscopic viewpoint. It is modeled as a compact time-dependent scatterer connected to leads where the particles move freely. This approach provides a description of charge transport, expressed by a formula due to Büttiker, Thomas and Prêtre, as well as of dissipation and of entropy and noise currents in terms of static scattering data. The charge transported in a cycle is quantized in special cases only. The scattering approach to quantum pumping is naturally described in geometrical terms.

A comparison between the two approaches becomes possible after truncating the potential to a finite length, while the rest of the line gives rise to the leads. The system becomes then amenable to the scattering approach. In the limit where the length of the scatterer tends to infinity, the condition for quantization is attained and the two theories are shown to agree.

ZUSAMMENFASSUNG. Diese Dissertation behandelt Ladungstransport in Quantenpumpen, kompakten Geräten, die auf mesoskopischer Skala operieren, an mehrere Drähte angeschlossen und durch einen sich zeitlich periodisch verändernden Parameter bestimmt sind. In jedem Pumpzyklus transportieren sie Nettoladung von einem Draht zu einem anderen.

Es gibt verschiedene Theorien für die Beschreibung von Quantenpumpen, die von verschiedenen Idealisierungen des Geräts stammen. In dieser Arbeit konzentrieren wir uns auf zwei Theorien des Pumpens im adiabatischen Bereich.

Im topologischen Zugang wird eine Quantenpumpe vom mikroskopischen Standpunkt aus betrachet. Sie wird durch ein unendlich ausgedehntes Potential mit periodischer Zeitabhängigkeit modelliert. Das Potential muss eine Spektrallücke im instantanen Hamiltonoperator erzeugen, und die Fermienergie muss zu allen Zeiten des Zyklus in einer solchen Lücke liegen. Die Ladung, die durch einen Referenzpunkt während eines Zyklus transportiert wird, ist dann ganzzahlig. Diese Quantisierung ist topologischer Natur: Der Ladungstransport wird mit der Chernzahl eines Faserbündels identifiziert. Thouless fand dieses Ergebnis für räumlich periodische Potentiale mit einem Kanal. Wir erweitern es für nicht-periodische Potentiale mit mehreren Kanälen.

Im Streuzugang wird die Pumpe vom makroskopischen Standpunkt aus betrachtet. Sie wird als ein kompaktes zeitabhängiges Streuzentrum, das mit idealen Drähten verbunden ist, modelliert. Dieser Zugang gibt eine Beschreibung des Ladungstransports durch eine Formel von Büttiker, Thomas und Prêtre, und ausserdem von Dissipation, Entropie- und Rauschströmen anhand von statischen Streudaten. Die Ladung, die in einem Zyklus transportiert wird, ist nur in Spezialfällen quantisiert. Der Streuzugang zu Quantenpumpen wird natürlicherweise in geometrischer Sprache formuliert.

Zwischen den beiden Formulierungen wird ein Vergleich möglich, sobald man das Potential auf endlicher Länge abschneidet, während die beiden restlichen Teile die Drähte darstellen. Dieses System kann man dann mit dem Streuzugang untersuchen. Im Limes von unendlich ausgedehntem Streuzentrum wird die Quantisierungsbedingung erreicht und wir zeigen, dass die beiden Theorien übereinstimmen.

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Contents

CHAPTER 1

Introduction

Pumping devices have been known to mankind since several centuries and are present in people's everyday life, think for instance of the Archimedean screw and of bicycle pumps. Abstractly speaking a pump is a periodically time-dependent device transporting matter from some reservoir to some other, the reservoirs being such that if the pump does not operate no transport takes place. Pumps that transport electrons exploiting their wave nature are known as quantum pumps. These are mesoscopic devices connected to several leads, controlled by some parameters varying periodically in time and achieving a net transport from one lead to another at each cycle of the pump. Each lead may have several channels, representing for instance transversal modes. If the typical frequency at which the pump operates is small with respect to other energy scales present in the system, the pump is called adiabatic. Some theories that describe quantum pumping have been constructed. The emphasis in this work will be on two descriptions of adiabatic pumping: the topological approach, originated by the work of Thouless, and on the scattering approach, which was started by the work of Büttiker, Thomas and Prêtre. One further approach, which we will describe only shortly, has to be mentioned. It is the theory of full counting statistics, initiated by Levitov and Lesovik.

The topological approach considers the pump microscopically, and it describes it as an infinitely extended electric potential, with a periodic time dependence. The system described is an insulator: the potential has to produce a spectral gap, and the Fermi energy has to lie in this gap at any time during the cycle. The charge transported in a cycle of the pump is found to be quantized, and this quantization is ascribed to topological reasons, whence the name of the approach. In the scattering approach the pump is considered from a macroscopic viewpoint, as a compact scatterer connected to leads where the particles move freely. There is therefore no spectral gap in the Hamiltonian. Remarkably, the adiabatic time dependence of the pump has as a consequence the fact that charge transport depends on static scattering data only. The charge transported in a cycle is found not to be quantized in general, although a particular class of pump operations is singled out by quantization of charge transport. These are called optimal pumps, and also have vanishing noise.

The two points of view, though different, have a point of contact: if the scatterer is taken as a finite but long portion of the infinitely extended potential, one would want the two theories to agree. If this is the case, one could design experimentally realizable

devices, implementing the topological mechanism of quantization of charge transport. The main result of this work is that this is actually the case: in the situation described above, and in the limit where the length of the finite portion of the potential tends to infinity, the results of the two theories agree. A physical argument for this fact is the following. The energies in the gap, appearing in the spectrum upon truncation of the potential, correspond to states well localized in the leads. In the adiabatic limit, their contribution to the current is proportional to their probability to tunnel through the finite portion of the potential. As the potential describes an insulator, the tunnel probability is exponentially small in the length of the portion. The "distance" between the actual system and the abstract idealization given by the modeling of the topological approach, is therefore not the infinite difference between the length of the potentials, instead it is the value of the physically relevant quantity, the transmission probability at the Fermi energy. As this is very small, the abstraction of topological approach captures a very interesting element of reality: the quantization of the charge transport.

Summary of the Thesis

The theories we are going to compare in this work both treat independent electrons. In Chapter 2 we present the topological approach to pumping. The pump is modelled as an infinitely extended potential, whose time dependence is assumed periodic and slow. The system is assumed to be insulating all along the cycle: the Hamiltonians have to have a spectral gap containing the Fermi energy during the entire period of the pump. The temperature is assumed to be $T = 0$.

The quantity under study is the charge transported through a reference point x_0 during a cycle. We will first describe the work of Thouless, where the charge transport is found to be an integer, under the additional assumption that the potential is spatially periodic. This is related to the fact that it is the Chern number of a fiber bundle, the quantization being therefore of topological nature.

We will then proceed to the first result of this work: the generalization of quantization of charge transport to arbitrary potentials, allowing a multi-channel setting. We will describe in detail the fiber bundle underlying the quantization.

In Chapter 3 we will describe the scattering approach to pumping. In the scattering approach the pump is modelled as a slowly time-dependent scatterer connected to several leads, where the particles move freely. The state of the particles in the leads is described by a density matrix $\rho(E)$, with ρ the Fermi function. The chemical potential and the temperature are the same in all leads.

The current, the dissipation and the currents of entropy and noise are described by formulae which are local in time. The formula for the charge transport, due to Büttiker, Thomas and Prêtre, is called the BPT formula. It is, surprisingly, valid even for $T = 0$, where the energy scale defined by the adiabatic pump $\hbar\omega$ (ω is the operational frequency of the pump) is big with respect to the energy scale $k_B T$. This is the case for

the formula describing dissipation, too. In contrast, the formulae for noise and entropy currents are valid only for $\hbar\omega \ll k_B T$.

An interesting feature of the scattering approach to quantum pumping is that it allows a geometrical interpretation: we will describe the formula for the four quantities introduced above in geometrical terms. We will close the chapter with some examples.

In Chapter 4 we will prove the equivalence between the topological and scattering approaches to pumping: in the limit of a long truncated pump the predictions of the two theories agree. We will show this first for the case of a periodic one channel potential. This will highlight the main points in the proof of the general case of non-periodic n-channel potentials.

Throughout this work we will have chosen units such that $2m_e = e = k_B = \hbar = 1$.

CHAPTER 2

The topological approach to pumping

In this chapter we describe the topological approach to quantum pumping. In this approach the system is modelled as a gas of non-interacting fermions subject to an infinitely extended potential, whose shape varies slowly and periodically in time. The temperature of the system is assumed to be $T = 0$. The main assumption about the potential is that it produces an energy gap, and the Fermi energy is supposed to lie in such a gap at every time, so that the system describes an insulator. The quantity of interest is the current, or more precisely its integral over a time cycle, the charge transport ascribed to the pump. As the time dependence of the Hamiltonian is slow, it makes sense to decompose the contributions to the current in powers of ω, the typical frequency of the pump. At order ω^0, the state of the electrons is the Fermi sea, and the currents are persistent currents, which, as we will see, disappear in the case under study. This is not the case at order ω^1, where electrons in the Fermi sea may take virtual transitions to the unoccupied bands, producing a current. As the duration of a cycle is ω^{-1}, the charge transport is of order one, and the system achieves pumping in the adiabatic limit. The amazing discovery of Thouless [**65**] is that in this situation the charge transport is given by an integer number, provided that the potential is space periodic. The reason for this quantization is of topological nature: Thouless shows that the charge transport is given by the first Chern number of a fiber bundle.

As said, this result holds in the adiabatic limit, where the frequency ω of the pump is small, and the reason for the assumption about the Fermi energy is that it is needed in order to apply standard adiabatic theory. This assumption is crucial for the construction of the topological approach, and for the quantization to hold. This seems not to be the case for the space periodicity of the potential, and in fact it is possible to drop this assumption and generalize the topological quantization of charge transport to non-periodic potentials and to an n-channel setting.

We now give a more detailed description of the model and of the results: the Hamiltonian

$$H(s) = -\frac{d^2}{dx^2} + V(x, s)\,, \tag{2.1}$$

acts on $L^2(\mathbb{R}_x, \mathbb{C}^n)$, where n is the number of channels (allowing for instance the wire under description to have many transversal modes). The potential $V = V(x, s)$ takes values in the $n \times n$ matrices, $M_n(\mathbb{C})$, is Hermitian, $V = V^*$, and periodic in time, $V(x, s + 2\pi) = V(x, s)$.

We study the evolution of the Fermi sea under the non-autonomous Hamiltonian $H(\omega t)$, $s = \omega t$ in the adiabatic limit $\omega \to 0$. To do this we assume that the Fermi energy $\mu > 0$ lies in a spectral gap for the entire cycle:

$$\mu \in \rho(H(s)) \qquad \forall s\,, \tag{2.2}$$

which allows the application of the adiabatic theorem of quantum mechanics [**12**]: let $P_0(s)$ be the spectral projection of $H(s)$ up to the Fermi energy, and $U_\omega(s, s_0)$ be the propagator for $H(\omega t)$; then

$$P(s) = U_\omega(s, s_0)(P_0(s_0) - \omega P_1(s_0))U_\omega(s, s_0)^* = P_0(s) + \omega P_1(s) + O(\omega^2)\,, \qquad (\omega \to 0) \tag{2.3}$$

with [**13**]

$$P_1(s) = -\frac{1}{2\pi} \oint_{\gamma(s)} R(s, z)[\dot{P}(s), P(s)]R(s, z)\, dz\,, \tag{2.4}$$

where $R(s, z) = (H(s) - z)^{-1}$ and $\gamma(s) \subset \mathbb{C}$ is a contour encircling the energies of occupied states. The expression (2.3) is the one-particle density matrix which has evolved from that of the Fermi sea, $P_0(s_0)$, after a gentle start of the pump. In fact such a start may be obtained from (2.1) by means of a smooth substitution $s' \mapsto s$ with $s' \mapsto s_0$, $(s \le s_0)$, and $s' = s$, (s' large). Then, in the new variable, $P_1(s_0) = 0$ by (2.4).

The quantity under study here is the charge transported through a point x_0 in a cycle (of duration $2\pi\omega^{-1}$). The current I is the rate of change of the charge contained in $x > x_0$ and hence given by the operator $I = \mathrm{i}[H(s), \theta(x - x_0)]$, which is independent of s. The charge transport is then given, in expectation value, as

$$\langle Q \rangle = \oint \mathrm{Tr}(IP(\omega t))dt = \oint \mathrm{Tr}(IP(s))\omega^{-1} ds\,, \tag{2.5}$$

where Tr denotes the trace over $L^2(\mathbb{R}_x, \mathbb{C}^n)$. Only two terms in (2.5) survive in the adiabatic limit: the first one, $\omega^{-1} \oint \mathrm{Tr}(IP_0(s))ds$, describing persistent currents, is actually potentially divergent in the limit. We show in Section 2 that this term vanishes (if V were real, this would follow trivially from time reversal invariance; however our hypothesis does not imply this, except for $n = 1$, and we shall argue otherwise). The second term describes therefore the charge transport in the adiabatic limit:

$$\langle Q_T \rangle := \oint \mathrm{Tr}(IP_1(s))ds\,. \tag{2.6}$$

Thouless [**65**] has calculated the charge transport (2.6) with the further assumption that the potential V is space periodic (and for one channel) and has noticed that $\langle Q_T \rangle$ can assume only integer values, as the formula he derived for the charge transport manifests itself as the Chern number of a fiber bundle. We present this result in Section 1. In Section 2 we generalize this result dropping the assumption about space periodicity of the potential and allowing the model to have n channels. This includes in particular the vanishing of persistent currents, which is not trivial any more, and the derivation of a

formula exhibiting (2.6) as the Chern number of a fiber bundle, which will be described in detail.

1. The case of Bloch Hamiltonians

This section is devoted to the description of the results obtained by Thouless in [**65**]. The setting is the one described in the introduction to this chapter, with H a single-channel Hamiltonian and the further assumption that the potential V is space periodic, $V(x+1,s) = V(x,s)$. The Hamiltonian is then a direct integral $H = \int^{\oplus} dk\, H_k$ [**51**] and the problem becomes amenable to an analysis in term of Bloch waves.

Thouless provides two descriptions of charge transport: in the first one $\langle Q_T \rangle$ is expressed as a sum of integrals over the Brillouin zone, the sum being over occupied bands; in the second one the integral over quasi-momentum k is substituted by a contour integral in the complex energy plane, the contour of integration surrounding the occupied energies. The second description is better suited to understand both the generalization to n channels and general potentials, and the equivalence with the scattering approach. In both description the topological quantization of charge transport is manifest: the integrals in the two-formulae are Chern numbers.

After the discussion of these results, we present some works which have been inspired by [**65**]; in particular we discuss [**47**]: the fact that the periodicity of the potential is not necessary for the quantization of charge transport was already stated there, but this is done approximating the general potential with periodic ones, and only these are associated to fiber bundles.

We proceed now to the presentation of the two descriptions of charge transport: the adiabatic analysis produces the following formula for the expectation value of the space average of the instantaneous current:

$$\langle I \rangle(s) = \frac{\mathrm{i}}{\pi} \oint dz \int_0^1 dx \int_{-\infty}^{+\infty} dy\, \frac{\partial}{\partial x} G_s(x,y;z) \frac{\partial}{\partial s} G_s(y,x;z), \tag{2.7}$$

where G_s is the Green function for the Hamiltonian $H(s)$ (the integrand in (2.42) below is the instantaneous current across a reference point x_0 in the general case ($x_0 = 0$ there): the choice of different reference points, and as a consequence the choice to average over reference points, produces different instantaneous currents, as physical reasoning suggests, but this dependence is lifted after integration over a cycle).

The Bloch waves $\psi_{nks}(x)$ are the solutions of the time-independent Schrödinger equation

$$H(s)\psi_{nks} = E_{ns}(k)\psi_{nks}\,, \qquad (E \in \mathbb{R})\,, \tag{2.8}$$

with Bloch boundary condition

$$\psi_{nks}(x+1) = \mathrm{e}^{\mathrm{i}k}\psi_{nks}(x)\,, \qquad (k \in \mathbb{R} \mod 2\pi) \tag{2.9}$$

and normalized with respect to the inner product

$$\langle \phi, \psi \rangle = \int_0^1 dx\, \overline{\phi}(x)\psi(x)\,,$$

(the index $n = 1, 2, ..$ labels the bands). Thouless writes (2.7) in term of Bloch waves as (dropping the dependence on s):

$$\langle I \rangle = \frac{1}{\pi} \sum_{n\, m} \int dk (E_n(k) - E_m(k))^{-1} \big(\langle \frac{\partial \psi_{nk}}{\partial x}, \psi_{mk} \rangle \langle \psi_{mk}, \frac{\partial \psi_{nk}}{\partial s} \rangle + \langle \frac{\partial \psi_{nk}}{\partial s}, \psi_{mk} \rangle \langle \psi_{mk}, \frac{\partial \psi_{nk}}{\partial x} \rangle \big)\,,$$

where the sum runs over occupied bands for n and empty bands for m. This, after integration over a cycle, is shown to give

$$\langle Q_T \rangle = \sum_{n : E_n < \mu} \frac{\mathrm{i}}{2\pi} \oint ds \oint dk \big(\langle \frac{\partial \psi_{nks}}{\partial s}, \frac{\partial \psi_{nks}}{\partial k} \rangle - \langle \frac{\partial \psi_{nks}}{\partial k}, \frac{\partial \psi_{nks}}{\partial s} \rangle \big)\,. \tag{2.10}$$

Each term of this sum is an integer, being the Chern number of the $U(1)$ fiber bundle ψ_{nks} over the torus $S^1_s \times S^1_k$. This number reflects the obstruction to continuously choosing the phase of ψ_{nks} on the entire torus. These integrals bear a formal resemblance with the ones appearing in the formula [**68**] for the quantum Hall conductance in systems with a periodic substrate potential, where the torus of integration is the magnetic Brillouin zone $S^1_{k_1} \times S^1_{k_2}$.

The second description of charge transport is obtained in [**65**] from the first one by analytic continuation, and is written in term of the functions $\psi_\pm(x)$ defined as follows: the time-independent Schrödinger equation

$$H(s)\psi_\pm = z\psi_\pm\,, \tag{2.11}$$

seen as a differential equation, clearly still has solutions for $z \in \rho(H(s))$. These solutions tend to zero at one spatial infinity and are unbounded at the other, we call them $\psi_\pm(x)$ for $\psi_\pm \to 0$, $x \to \pm\infty$ (not displaying the dependence on z, s in the notation). In term of these functions the charge transport is

$$\langle Q_T \rangle = \oint_\gamma dz \oint_{S^1} ds \big(\langle \frac{\partial \psi_-}{\partial z}, \frac{\partial \psi_+}{\partial s} \rangle - \langle \frac{\partial \psi_-}{\partial s}, \frac{\partial \psi_+}{\partial z} \rangle \big)\,. \tag{2.12}$$

for $\psi_\pm$ chosen locally smooth in (z, s) and satisfying $\langle \psi_-, \psi_+ \rangle = 1$, and γ a contour surrounding the occupied energies. In the next section we will provide a derivation of (2.12) directly from (2.7), without going through the first description (see the proof of Theorem 1, part *ii*) and the remark in Paragraph 2.2), and a description of the bundle underlying it.

The expression (2.12) can be calculated in a simple and elegant way: it is the net number of nodes of the solution ψ_+ at the Fermi energy going through a point x_0 in space during a cycle (this number clearly does not depend on x_0). We give here a short

outline of the argument for this fact, because the ideas in this argument are very helpful to understand the proof of the equivalence to the scattering approach. It is possible to fix the phase of ψ_+ by requiring the value of $\psi_+(x_0)$ to be real and positive; this choice works for the entire torus $\gamma \times S^1$, up to the points (z, s) where $\psi_+(x_0) = 0$. The integral (2.12) then reduces to a sum of winding numbers around these singular points. These points must have $z = \mu$, because $\psi_+(x_0) = 0$ implies that $\psi_+(x)$ is an eigenfunction (with eigenvalue z) to the operator $H(s)$ on $L^2([x_0, x_0+1])$ with Dirichlet boundary conditions, a self-adjoint operator. The winding number around a singular point is generically the sign of $-\partial_z\psi_+(x_0)\partial_s\psi_+(x_0)$. The calculation

$$
\begin{aligned}
(2.13) \quad -\frac{\partial\psi_+}{\partial x}(x_0)\frac{\partial\psi_+}{\partial z}(x_0) &= \int_{x_0}^{\infty} dx\,(\frac{\partial\psi_+}{\partial x}(x)\frac{\partial\psi_+}{\partial z}(x) - \psi_+(x)\frac{\partial^2\psi_+}{\partial x\partial z})' \\
&= \int_{x_0}^{\infty} dx\,(\psi_+(x))^2 > 0
\end{aligned}
$$

(the first equality follows from $\psi_+(x_0) = 0$, the second from (2.11)) gives a relation between the sign of $\partial_z\psi_+(x_0)$ and the sign of $\partial_x\psi_+(x_0)$, thus implying that the contribution of a singular point depends only on the direction in which the node of ψ_+ traverses x_0.

Example: Let V be a potential with constant shape that translates in time $V(x, s) = V(x - s/2\pi)$. Fix n such that the band z_n is occupied (n is henceforth dropped from the notation).

For $s = 0$ we can choose $\tilde{\psi}_{k0}(x)$ (solving (2.8), (2.9)) continuously for $k \in [0, 2\pi]$; we then know that $\tilde{\psi}_{2\pi 0}(x) = \mathrm{e}^{\mathrm{i}\alpha}\tilde{\psi}_{00}(x)$.

The definition

$$
\begin{aligned}
\psi_{k0}(x) &= \mathrm{e}^{-\mathrm{i}\frac{\alpha}{2\pi}k}\tilde{\psi}_{k0}(x) \\
\psi_{ks}(x) &= \psi_{k0}(x - s/2\pi)
\end{aligned}
$$

now implies

$$
\begin{aligned}
&\psi_{2\pi 0}(x) = \psi_{00}(x) \\
&\psi_{2\pi s}(x) = \psi_{2\pi 0}(x - s/2\pi) = \psi_{00}(x - s/2\pi) = \psi_{0s}(x)
\end{aligned}
$$

i.e. the phase of ψ_{ks} has been chosen continuously on the cylinder obtained from the torus $S^1_t \times S^1_k$ cutting along $s = 0$. The n-th integral in (2.10) can be calculated with Stokes theorem:

$$
\oint_{s=2\pi} dk\langle\psi_{ks}|\frac{\partial\psi_{ks}}{\partial k}\rangle - \oint_{s=0} dk\langle\psi_{ks}|\frac{\partial\psi_{ks}}{\partial k}\rangle\,.
$$

As

$$
\psi_{k2\pi}(x) = \psi_{k0}(x - 1) = \mathrm{e}^{-\mathrm{i}k}\psi_{k0}(x)
$$

(by (2.9)) the difference between the two integrals is $-2\pi\mathrm{i}$, and the charge transport (2.10) is equal to the number of occupied bands (this is the result that follows by Galilean invariance, as each band carries one unit of charge per unit cell).

According to the second description of $\langle Q_T \rangle$, the charge transport is equal to the number of nodes of $\psi_+(x)$ (at the Fermi energy) in a space period; this is equal to the previous description by a Sturm-Liouville like result. Further calculations of the charge transport for concrete models can be found in [**45**].

This work of Thouless was at the origin of much theoretical and experimental interest. It is considered to have been the first description of a quantum pump, and the expressions "Thouless pump" or "Thouless mechanism" often designate the possibility of achieving transport in an insulating regime by applying a time-dependent drive. The fact that quantization is ascribed to topological reasons may suggest that it should survive in a less idealized setting: if the infinite potential appearing in the description above is truncated to a finite interval, adding free leads at the truncation ends, the spectral gap closes. One can however argue that energies in the gap are attributed to states which are localized in the leads, and this should contribute to the current only through their tunnel probability, which has an exponential dependence on the length of the interval. An important consequence of the equivalence shown in Chapter 4 is the mathematical justification of this argument: when the length of the interval grows, the prediction of the topological theory agrees with the one of the scattering approach to pumping, which is the one suited for gapless open pumps. Also the effects of non-adiabaticity may be quantified [**54**]. This way one can design pumps, which implement the topological mechanism of quantization [**46, 64**]. On the other hand, the spectacular quantization of charge transport seen in experiments, as for instance [**56, 55, 25, 33, 15**], applying Thouless mechanism for pumping, is not due to the topological mechanism. In these experiments a potential wave slides through the sample, transporting electrons that take place in the minima of the wave. The mechanism for the quantization of transport [**49, 27**] is that the strong Coulomb repulsion fixes the number of electrons that occupy a potential minimum, and is therefore due to the interaction between electrons, whereas topological quantization already holds in the independent electrons approximation.

Experimental [**63**] and theoretical effort has been put into understanding adiabatic quantum pumping in open systems. This has produced the scattering approach to pumping [**22, 16**], and the theory of full counting statistics [**36, 35, 2, 29**] (the next chapter is devoted to the description of the scattering approach to pumping, with a brief section devoted to the description of full counting statistics). In this regime, the transported charge is not quantized as a rule, and interesting questions are raised on the nature of dissipation in pumping [**8, 10, 41**]. Although the charge transport is not quantized in general, we will see in the next chapter that one can geometrically characterize a class of pump operations with quantized charge transport. In this cases the charge transport is not only an integer in expectation value, but it also has vanishing

variance, so that the transport of charge is a fixed integer for every cycle of the pump. It has however to be cautioned that the mechanism for quantization is not the one described above and is not of topological nature (see Section 3). One can again analyse the quantization obtained in the experiments cited above, and see [**1, 23**] that it is at least partially understandable without referring to the Coulomb interaction between the electrons.

Thouless' work inspired [**31**], which in turn was the origin of a relevant progress in the theory of polarization in crystalline solids. The authors calculate the polarization change caused by an adiabatic change of the Hamiltonian $H(\lambda)$, and relate this quantity to Berry's phase [**14, 58**], or more precisely to Zak's phase [**71, 40**]. The change in the polarisation in direction α (provided the Hamiltonian $H(\lambda)$ is insulating for every value of λ, where λ runs from 0 to 1, which is again needed for the application of the adiabatic theorem) is found to be, in close analogy to (2.10),

$$\Delta P_\alpha = \frac{1}{8\pi^3 i} \sum_n \int d^3k \int_0^1 d\lambda \big(\langle \frac{\partial u_k}{\partial k_\alpha}, \frac{\partial u_k}{\partial \lambda} \rangle - \langle \frac{\partial u_k}{\partial \lambda}, \frac{\partial u_k}{\partial k_\alpha} \rangle \big) ,$$

where the k integral is over the Brillouin zone, the sum runs over occupied bands and $u_k(x) = \psi_k(x) \mathrm{e}^{-\mathrm{i}kx}$ is the periodic part of the Bloch wave $\psi_k(x)$ (the reason for the appearing of ψ_k and not u_k in (2.10) is that the x matrix elements produced by ∂_k upon the substitution disappear after time integration if the change in the Hamiltonian is periodic, as they may be written as a total time derivative). Stokes' theorem then implies

$$\Delta P_\alpha = P_\alpha^{(1)} - P_\alpha^{(0)} \tag{2.14}$$

$$P_\alpha^{(j)} = \frac{i}{8\pi^3} \sum_n \int dk \langle u_k^{(j)}, \frac{\partial u_k^{(j)}}{\partial k_\alpha} \rangle \tag{2.15}$$

as the contribution of the line integrals in direction $d\lambda$ cancel by periodicity of ψ_k, and therefore of $\langle u_k, \partial u_k / \partial \lambda \rangle$, (as a function of k) over the Brillouin zone. The terms in the sum in (2.15) are closely related to the Zak phase of the n-th band. Using these equalities the authors were able to obtain the piezoelectric tensor of GaAs from first principle calculations. If the Hamiltonian returns to the initial value at the end of the deformation, Thouless' topological quantization result directly implies $\Delta \vec{P} = \frac{1}{\Omega} \sum_n \vec{R}_n$, where $\vec{R}_n$ are vectors in the direct lattice of the crystal. This means one could hope to define the total polarization (modulo vectors in the direct lattice) through (2.15). This makes physical sense [**31**], as the polarization defined this way is in relation to the bound charge σ accumulating at a surface of orientation $\hat{n}$ via the equality $\sigma = \vec{P} \cdot \hat{n}$.

A nice illustration of the theory is given in [**6**], where using this description of polarization the piezoelectricity of Harper models was classified with the help of Chern numbers. Further developments are described e.g. in [**61, 60, 52**].

Topologically quantized quantities have been recognised in different systems in condensed matter physics, such as circulation quantization in superfluids, flux quantization and the Josephson effect in superconductors and the quantum Hall effect. The obvious reference is [**67**]. A field where topological quantization plays a major role is obviously the Quantum Hall effect. In fact the explanations of the integer Quantum Hall effect given by Laughlin [**32**] and Streda [**62**] share a topological flavour [**66**]. In particular, an abstraction of Laughlin's argument can be made [**3**] such that it leads to a topological interpretation of the quantized Hall conductance: σ_H is found to be a Chern number. In this construction the Hall probe is represented by a two dimensional structure where

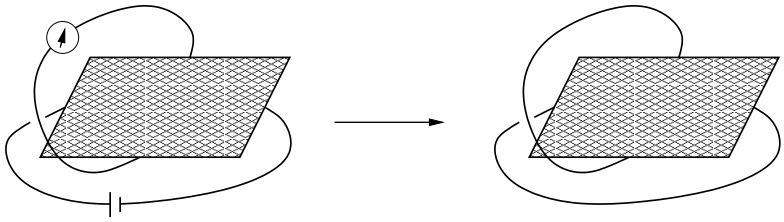


FIGURE 1. The usual quantum Hall setting of a two dimensional sample with an applied voltage and an ammeter measuring current in the normal direction, is substituted by the one on the right, where the ammeter is represented by a time-independent flux threading the current ring and monitoring the current and the voltage is produced by a time-dependent flux threading the voltage ring.

the two rings are threaded by magnetic fluxes. The first flux changes adiabatically in time and produces the voltage, the second represents the ammeter. As the Hamiltonian of the system is periodic in the fluxes (with period Φ_0, the flux quantum), the parameter space is a torus. The Hall conductance (averaged over the flux Φ in the ammeter ring), is the Chern number of the $U(1)$ bundle $|\psi_0\rangle$ over this torus ($|\psi_0\rangle$ is the ground state of the Hamiltonian associated to a given flux). Quantization via Chern numbers had first been recognized for the Quantum Hall effect in [**68**], where topological quantization for the Hall conductance is shown for Bloch Hamiltonians, and the formula for σ_H has a striking formal equivalence with (2.10). This has been later generalized to more general Hamiltonians, allowing impurities and many body interactions, in [**48**], which shares much of the structure with [**3**], although the formulation of the latter seems more elegant as the geometrical nature of the problem is more apparent.

In fact, the similarities between (2.10) and the equation manifesting the quantization of σ_H are not just formal, as the time dependence in the potential underlying (2.10) may come from the Galilei transformation cancelling the electric field in a Quantum Hall sample (see Figure 2). As the Galilean boost velocity is proportional to the electric field, the limit of vanishing electric field, in which the conductance is evaluated, is equivalent to the adiabatic limit taken to derive (2.10). Generalizing the results of [**65**] to non-periodic potentials has therefore the same flavour as the generalization for Hall

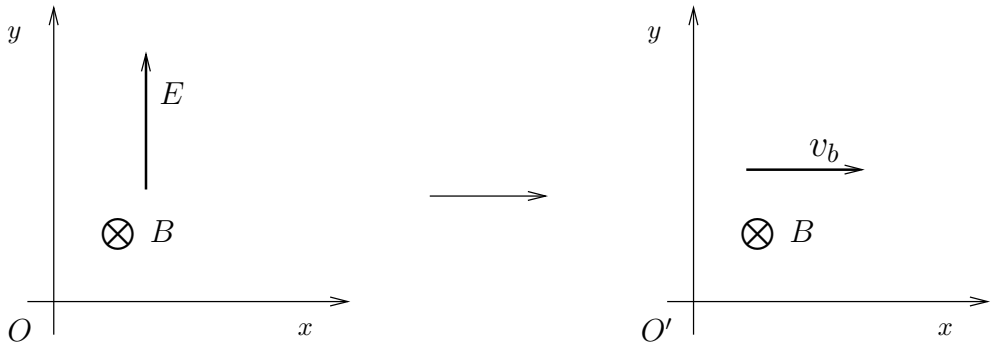


FIGURE 2. A Quantum Hall sample (left) with a periodic substrate potential $V(x)$ in reference frame O. In O', related to O by a Galilei transformation with boost velocity $v_b = E/B$, the electric field vanishes. The substrate potential obtains a time dependence $V'(x,t) = V(x - v_b t)$.

Hamiltonians described above. This leads us to [**47**], where precisely this generalization is done: the quantization of particle transport is generalized to non-periodic many body potential. We now describe this work and comment on the difference with our generalization of the work of Thouless at the end.

The Hamiltonian

$$H(s) = \sum_{i=1}^{N} \big(\frac{\partial^2}{\partial x_i^2} + V(x,s) \big) + \sum_{i>j}^{N} V(x_1 - x_j)$$

is now a many body Hamiltonian, and $V(x,s) = V(x,s+1)$ has no prescribed space periodicity. The assumptions on the Hamiltonian are the presence of an energy gap between the ground state and the first excited state (needed for the application of the adiabatic theorem), and the exponential fall-off of the Green function. The Hamiltonian acts on states satisfying the periodic boundary conditions

$$\psi(x_1, \ldots, x_i + L, \ldots, x_N) = \psi(x_1, \ldots, x_i, \ldots, x_N)\,,$$

and the charge transport is calculated in the thermodynamic limit $N \to \infty$, $L \to \infty$ with N/L constant.

The idea is to compare the charge transport to an averaged value, the average being taken over generalized periodic boundary conditions

$$\psi(x_1, \ldots, x_i + L, \ldots, x_N) = \mathrm{e}^{\mathrm{i}\alpha L} \psi(x_1, \ldots, x_i, \ldots, x_N)\,,$$

as the averaged quantity is easily related to a Chern number, and is therefore integer.

The charge transport for a given boundary condition α is found by application of the adiabatic theorem, and is most compactly written in term of the functions $|\psi_\alpha\rangle = \mathrm{e}^{-\mathrm{i}\alpha(x_1+\ldots+x_n)}|\psi_\alpha^{(0)}\rangle$ (where $|\psi_\alpha^{(0)}\rangle$ is the many body ground state with boundary condition

α):

$$\langle Q\rangle_\alpha = \frac{\mathrm{i}}{L}\oint_{S^1} ds\big(\langle\frac{\partial\psi_\alpha}{\partial s},\frac{\partial\psi_\alpha}{\partial\alpha}\rangle - \langle\frac{\partial\psi_\alpha}{\partial\alpha},\frac{\partial\psi_\alpha}{\partial s}\rangle\big)\,.$$

The result is that the difference between the charge transport and the averaged value vanishes in the thermodynamic limit

$$\langle Q\rangle_0 - \frac{L}{2\pi}\int_{-\pi/L}^{\pi/L} d\alpha\langle Q\rangle_\alpha \to 0 \qquad (L\to\infty\,(TD))\,.$$

The averaged quantity

$$\overline{\langle Q\rangle}_\alpha = \frac{\mathrm{i}}{2\pi}\int_{-\pi}^{\pi} d\beta\oint_{S^1} ds\big(\langle\frac{\partial\psi_\alpha}{\partial s},\frac{\partial\psi_\alpha}{\partial\alpha}\rangle - \langle\frac{\partial\psi_\alpha}{\partial\alpha},\frac{\partial\psi_\alpha}{\partial s}\rangle\big) \qquad (\beta = L\alpha) \tag{2.16}$$

is recognised as a Chern number. In the case of non interacting electrons, ψ_α is a Slater determinant of the u_α (again, the periodic part of the Bloch waves), and transport is described by a sum over occupied states, which approximate the continuum spectrum in the limit $L\to\infty$. If the potential is periodic one gets back (2.10) by substituting the u_α with the Bloch wave functions, what is possible because the supplementary x matrix elements vanish after time integration.

The differences between this construction and our generalization to arbitrary non-periodic potentials are the following: on the one hand our generalization is only for one particle Hamiltonians, on the other hand, in strong contrast to the one just presented, it refers to the infinite system. In [**47**] the system is approximated by finite ones, charge transport is calculated, averaged over boundary conditions, in the approximants, the geometric structure pertains to the approximants only and is introduced by the averaging procedure. In our generalization the charge transport is calculated, exactly, in the infinite system, and more importantly the geometric construction associates a bundle directly to the infinite system.

2. Generalization to non periodic n-channel potentials

As announced, it is not necessary to require periodicity of the potential in order to obtain topological quantization of charge transport. This is the content of this section: we present the generalization of the result by Thouless to n-channel potentials.

In this setting the Hamiltonian at a fixed time is not time-reversal invariant. The vanishing of persistent currents is thus no longer trivial and is the content of Theorem 1. Topological quantization of charge transport is stated in Theorem 2, where $\langle Q_T\rangle$ is written in a form manifesting it as the Chern number of a bundle. The basis manifold is, as in (2.12), the torus $\gamma\times S^1_s$, with γ a closed curve lying in the resolvent set. For every energy in γ, there are n unbounded solutions regular at either $x=\pm\infty$, and the fibers of the bundle are described in term of those.

The description of the fibers is necessary to state Theorem 2, and will open Paragraph 2.1. The statement of the theorems will follow. Paragraph 2.2 provides a detailed

description of the fiber bundle and of the connection underlying Theorem 2. The last paragraph of the section is then devoted to the proofs of these results.

2.1. Statement. In search of a generalization of (2.10) one has to identify the objects analogous to the $\psi_\pm$. This is understood as follows: the (kets) ψ_+ in (2.10) identify the linear space of solutions to the Schrödinger equation regular at $x = +\infty$, and the (bras) ψ_- identify the linear space of solutions to the adjoint Schrödinger equation decaying at $x = -\infty$. One therefore has to find objects identifying the n-dimensional linear spaces of solutions of the Schrödinger equation (respectively of the adjoint one) regular at the corresponding end. Such an object is constructed taking n independent solutions and grouping them in a matrix. The sets of such matrix-valued functions will carry a natural $\mathrm{GL}(n)$ action, corresponding to a change of the basis of the linear space of solutions. One also has to define a bilinear form between elements of these two sets, as the lack of periodicity takes the natural choice of the scalar product away.

We now define these objects: we have to describe the sets of solutions φ to the Schrödinger equation

$$H(s)\varphi = z\varphi \tag{2.17}$$

for z in the resolvent set of $H(s)$: let us for simplicity assume $V(\cdot, s) \in L^\infty(\mathbb{R}_x, M_n(\mathbb{C}))$ with C^1-dependence on $s \in S^1 := \mathbb{R}/2\pi\mathbb{Z}$; then, for any $z \in \rho(H(s))$, (2.17) is in the limit-point case at $x = +\infty$ (see [**37**] or [**24, 34**]), meaning that as an ordinary differential equation it has n linearly independent solutions which are square-integrable at $x = +\infty$. We may thus introduce a family of sets, parametrized by $z \in \rho(H(s))$ and $s \in S^1$, consisting of matrix-valued solutions $\psi(x) \in M_n(\mathbb{C})$ of the Schrödinger equation

$$-\psi''(x) + V(x, s)\psi(x) = z\psi(x)\,, \tag{2.18}$$

which are regular in the sense that for any $x \in \mathbb{R}$

$$\psi(x)a = 0,\ \psi'(x)a = 0 \ \Rightarrow\ a = 0\,, \qquad (a \in \mathbb{C}^n)\,. \tag{2.19}$$

It is:

$$S^+_{(z,s)} = \{\psi_+ | \psi_+ \text{ is a regular solution of (2.18)}, L^2 \text{ at } x = +\infty\}\,. \tag{2.20}$$

As a matter of fact such solutions tend to zero pointwise as $x \to +\infty$, together with their first derivatives. As will be explained in Paragraph 2.2 $S^+_{(z,s)}$ is the fiber at base point (z, s). Similarly, solutions $\tilde\psi(x) \in M_n(\mathbb{C})$ of the adjoint equation

$$-\tilde\psi''(x) + \tilde\psi(x)V(x, s) = z\tilde\psi(x) \tag{2.21}$$

act on row vectors $a \in \mathbb{C}^n$ as $a\tilde\psi(x)$, and we set

$$\tilde S^-_{(z,s)} = \{\tilde\psi_- | \tilde\psi_- \text{ is regular solution of (2.21)}, L^2 \text{ at } x = -\infty\}\,.$$

For later use we also introduce the families $S^-_{(z,s)}$, $\tilde{S}^+_{(z,s)}$ of solutions to (2.18), resp. (2.21) decaying at the opposite ends.

We now pass to the definition of the needed bilinear form: for any two differentiable functions ψ, $\tilde{\psi} : \mathbb{R} \to M_n(\mathbb{C})$ we define the Wronskian

$$W(\tilde{\psi}, \psi; x) = \tilde{\psi}(x)\psi'(x) - \tilde{\psi}'(x)\psi(x) \in M_n(\mathbb{C})\,. \tag{2.22}$$

It is independent of x if ψ and $\tilde{\psi}$ are solutions of (2.18), resp. of (2.21), in which case it is simply denoted as $W(\tilde{\psi}_-, \psi_+)$. As will be shown in the next paragraph, $\det W(\tilde{\psi}_-, \psi_+) \neq 0$ for $\psi_+ \in S^+_{(z,s)}$, $\tilde{\psi}_- \in \tilde{S}^-_{(z,s)}$.

We observe that $S^+_{(z,s)}$ carries a transitive right action of $\mathrm{GL}(n) \ni T$,

$$\psi_+(x) \mapsto \psi_+(x)T\,, \tag{2.23}$$

while $\tilde{S}^-_{(z,s)}$ carries a left action,

$$\tilde{\psi}_-(x) \mapsto T\tilde{\psi}_-(x)\,.$$

We thus have a bijective relation between $\psi_+ \in S^+_{(z,s)}$ and $\tilde{\psi}_- \in \tilde{S}^-_{(z,s)}$ such that

$$W(\tilde{\psi}_-, \psi_+) = 1\,. \tag{2.24}$$

As announced, there are no persistent currents:

THEOREM 1. *Assume (2.2). Then*

$$\mathrm{Tr}(IP_0(s)) = 0\,.$$

The charge transport is then described by

THEOREM 2.

$$\langle Q_T \rangle = \frac{\mathrm{i}}{2\pi} \oint_\gamma dz \oint_{S^1} ds\ \mathrm{tr}\big(W(\frac{\partial\tilde{\psi}_-}{\partial z}, \frac{\partial\psi_+}{\partial s}; x_0) - W(\frac{\partial\tilde{\psi}_-}{\partial s}, \frac{\partial\psi_+}{\partial z}; x_0)\big)\,, \tag{2.25}$$

where tr *denotes the matrix trace and the solutions $\psi_+ \in S^+_{(z,s)}$, $\tilde{\psi}_- \in \tilde{S}^-_{(z,s)}$ satisfying (2.24) are locally smooth in (z, s). Except for these conditions, the trace is independent of ψ_+, $\tilde{\psi}_-$, and the integral is it of x_0, too. Moreover, the r.h.s. is the first Chern number of a bundle described in the next paragraph.*

The proof of Theorem 2 relies on the following general result in adiabatic theory. Consider the usual quantum mechanical, adiabatic setting in presence of a spectral gap: a family of operators $H(s)$ depending smoothly on s and corresponding spectral projections $P(s)$ belonging to an interval $I(s)$ whose endpoints lie in the resolvent set $\rho\big(H(s)\big)$. Let $U_\omega(s, s_0)$ be the propagator for the non-autonomous Hamiltonian $H(s)$ with $s = \omega t$. Then

$$U_\omega(s, s_0)(P(s_0) + \omega P_1(s_0))U_\omega(s, s_0)^* = P(s) + \omega P_1(s) + O(\omega^2)\,, \qquad (\omega \to 0)$$

as explained above, with $P_1(s)$ as given by Eq. (2.4), see [**12**], Eq. (2.6) and [**13**], Eq. (2.10a). We find an alternate formula for P_1:

LEMMA 3. *In this setting, P_1 can be written as*

$$P_1(s) = -\frac{1}{2\pi} \oint_{\gamma(s)} R(s,z)\dot{R}(s,z)\, dz\,. \tag{2.26}$$

2.2. Topological and geometrical structure. We now describe the bundle P and the connection underlying Eq. (2.25). A fiber bundle is a differentiable manifold P, having locally the form of a product $M \times F$. M (a compact manifold) is called the basis, and F the (typical) fiber. An example is the tangent bundle $TM = \cup_{p\in M} T_pM$ with basis M and typical fiber $\mathbb{R}^m$, where m is the dimension of M. The splitting in basis and fibers is realized by the projection $\pi : P \to M$, the fiber at point $p \in M$ being $F_p = \pi^{-1}(x)$, and the local structure is given by the local trivialization (trivial meaning with the structure of a Cartesian product) $\phi_k^{-1} : \pi^{-1}(U_k) \to U_k \times F$, with U_k an open covering of the basis manifold. On $\pi^{-1}(U_k \cap U_l)$ the "change in coordinate" in the fibers is realized by the transition functions $T_{kl} : F \to F$, with $\phi_l^{-1} \circ \phi_k : (U_k \cap U_l) \times F \to (U_k \cap U_l) \times F = (\mathrm{Id}, T_{kl}(p))$. The transition functions all have to be elements of a (Lie) group $\mathcal{G}$, called the structure group of the bundle. They contain the information on how the fibers at different points are patched together, i.e. on the global structure of the bundle. If the typical fiber coincides with the structure group, which means that $\mathcal{G}$ acts transitively on $F_p = \pi^{-1}(p)$, the bundle is called a principal bundle.

We proceed with the description of the concrete bundle underlying (2.25): let $\mathcal{C} = C^1\big(\mathbb{R}, M_n(\mathbb{C})\big)$ be the space of matrix valued C^1-functions on $\mathbb{R}$. Let $\pi : P \to \mathbb{T}$ be the subbundle of $\mathbb{T} \times \mathcal{C}$ with base $\mathbb{T} = \gamma \times S^1$ (where $\mathbb{T}$ has the natural orientation $d\gamma \wedge ds$) and fibers $S^+_{(z,s)} \subset \mathcal{C}$:

$$P = \{((z,s), \psi \in \mathbb{T} \times \mathcal{C}) \mid \psi \in S^+_{(z,s)}\}\,.$$

It is a principal bundle w.r.t. the right action (2.23) of $\mathrm{GL}(n)$. This includes that $\mathrm{GL}(n)$ is its structure group. Indeed, for any sufficiently small open set $U \subset \mathbb{T}$ there is $x \in \mathbb{R}$ with

$$\det \psi_+(x) \neq 0 \tag{2.27}$$

for all $\psi_+ \in S^+_{(z,s)}$ and $(z,s) \in U$, see Lemma 5 in Chapter 4. This provides a local trivialization ϕ with

$$\phi^{-1} : \pi^{-1}(U) \to U \times \mathrm{GL}(n)\,, \quad \psi_+ \mapsto (z, s, \psi_+(x))\,.$$

The transition function $\phi_2^{-1} \circ \phi_1 : \mathrm{GL}(n) \to \mathrm{GL}(n)$ is multiplication from the left by the matrix $\psi_+(x_2)\psi_+(x_1)^{-1}$, which is clearly independent of $\psi_+ \in S^+_{(z,s)}$ and belongs to $\mathrm{GL}(n)$.

It is impossible to define the coordinate in the fiber in an intrinsic way: one has to refer to a local trivialization ϕ^{-1} or, equivalently, to a local section $\sigma : U_k \to P$ defining a reference point $e \in F_p$ in any fiber F_p, $p \in U_k$. The coordinate will then depend on the special section chosen and moreover cannot (as a rule) be defined globally, as non trivial principal bundles do not admit global sections. It is however possible to define changes in the fiber coordinates along any path $\gamma \subset P$ in an intrinsic way: this is done by the introduction of a connection $\mathcal{A} : TP \to \mathrm{Lie}(\mathcal{G})$, a Lie algebra valued one-form. For the changes to be described correctly, the connection has to produce the right answer for "vertical" paths $\gamma(\lambda)$ happening with constant base point p, i.e.

$$\mathcal{A}_{\gamma|_{\lambda=0}}(\gamma|_{\lambda=0} g) = g\,, \qquad g \in \mathrm{Lie}(\mathcal{G})\,. \tag{2.28}$$

Moreover, if $\gamma(\lambda)$ describes a parallel transport along $\pi(\gamma)(\lambda)$, the same should be true for γG, ($G \in \mathcal{G}$, where G acts only on the fibers). This is ensured by the condition

$$\mathcal{A}_{\gamma|_{\lambda=0}G}(\delta\gamma|_{\lambda=0} G) = G^{-1}\mathcal{A}_{\gamma|_{\lambda=0}}(\delta\gamma|_{\lambda=0})G\,. \tag{2.29}$$

The curvature $\mathcal{F} = D\mathcal{A}$ is the covariant derivative of the connection. Given a local section $\sigma_k : U_k \to \pi^{-1}(U_k)$, the connection one-form $\mathcal{A}$ defines (locally) a one-form on M, through the pull-back $\sigma_k^*\mathcal{A}$. It cannot be defined globally, as it depends on the choice of the local section. However, the trace of the curvature $\mathrm{tr}(\sigma_k^*\mathcal{F}) = d\,\mathrm{tr}(\sigma_k^*(\mathcal{A}))$ does not depend on σ_k, neither does $\mathrm{tr}(\sigma_k^*(\mathcal{A}) - \sigma_k^*(\mathcal{A}'))$, for any two connections $\mathcal{A}$, $\mathcal{A}'$; this means that $\mathrm{tr}(\mathcal{F})$ defines a two-form on M (not just on P), with $\mathrm{tr}(\mathcal{F}) - \mathrm{tr}(\mathcal{F}') = d(\mathrm{tr}(\sigma_k^*(\mathcal{A}) - \sigma_k^*(\mathcal{A}'))$ an exact two-form. As a consequence the Chern number of the bundle, defined as

$$C = \frac{\mathrm{i}}{2\pi}\int_{\mathbb{T}} \mathrm{tr}\,\mathcal{F}\,, \tag{2.30}$$

is independent on the choice of the connection $\mathcal{A}$. We consider connections of the following form. Let $B : \mathcal{C} \times \mathcal{C} \to M_n(\mathbb{C})$ be a bilinear form on $\mathcal{C}$ satisfying

$$B(\tilde\psi, \psi T) = B(\tilde\psi, \psi)T\,, \tag{2.31}$$

$$B(T\tilde\psi, \psi) = TB(\tilde\psi, \psi) \tag{2.32}$$

($\tilde\psi$, $\psi \in \mathcal{C}$, $T \in \mathrm{GL}(n)$). Moreover we assume that its restriction

$$B : \tilde S^-_{(z,s)} \times S^+_{(z,s)} \to \mathrm{GL}(n) \tag{2.33}$$

takes values $B(\tilde\psi_-, \psi_+)$ in the regular matrices (as shown below, an example is (2.22)). We may then consider the $\mathrm{gl}(n)$-valued one-form on P

$$\mathcal{A}_{\psi_+}(\delta\psi_+) = B(\tilde\psi_-, \psi_+)^{-1}B(\tilde\psi_-, \delta\psi_+)\,, \qquad (\delta\psi_+ \in TP)\,,$$

which is well-defined being independent of the choice of $\tilde\psi_- \in \tilde S^-_{(z,s)}$ by (2.32). It is a connection on P since it enjoys the defining properties (see (2.28), (2.29))

$$\mathcal{A}_{\psi_+}(\psi_+ t) = t\,, \qquad (t \in \mathrm{gl}(n))\,,$$
$$\mathcal{A}_{\psi_+ T}(\delta\psi_+ T) = T^{-1}\mathcal{A}_{\psi_+}(\delta\psi_+)T\,, \qquad (T \in \mathrm{GL}(n))$$

by (2.31). Given $\psi_+ \in S^+_{(z,s)}$ there is a unique $\tilde\psi_- \in \tilde S^-_{(z,s)}$ such that $B(\tilde\psi_-, \psi_+) = 1$, as can again be seen from (2.32). Then $\mathcal{A} = B(\tilde\psi_-, \delta\psi_+)$ and the trace of its curvature is

$$\mathrm{tr}\,\mathcal{F} = \mathrm{tr}\big(B(\frac{\partial\tilde\psi_-}{\partial z}, \frac{\partial\psi_+}{\partial s}) - B(\frac{\partial\tilde\psi_-}{\partial s}, \frac{\partial\psi_+}{\partial z})\big)dz\wedge ds\,.$$

We will use the bilinear

$$B(\tilde\psi, \psi) = W(\tilde\psi, \psi; x) = \tilde\psi(x)\psi'(x) - \tilde\psi'(x)\psi(x)\,,$$

whose restriction (2.33) is seen to be independent of x (though $\mathcal{A}$ may not be); then (2.30) coincides with the r.h.s. of (2.25), as announced in Theorem 2. It remains to verify $B(\tilde\psi_-, \psi_+) \in \mathrm{GL}(n)$. Any column vector solution $\varphi(x)$ of (2.18) is determined by $\varphi(0)$, $\varphi'(0) \in \mathbb{C}^n$. Similarly for any row vector $\tilde\varphi(x)$ solving (2.21). Their Wronskian

$$W(\tilde\varphi, \varphi) = \tilde\varphi(0)\varphi'(0) - \tilde\varphi'(0)\varphi(0)\,, \tag{2.34}$$

which now takes values in $\mathbb{C}$, clearly defines a non-degenerate bilinear form on $\mathbb{C}^{2n}$. Given $\psi_\pm \in S^\pm_{(z,s)}$, any solution φ can be expressed as

$$\varphi(x) = \psi_+(x)a_+ + \psi_-(x)a_- \tag{2.35}$$

with $a_\pm \in \mathbb{C}^n$, and $\varphi \equiv 0$ iff $a_\pm = 0$; similarly for $\tilde\varphi(x) = b_+\tilde\psi_+(x) + b_-\tilde\psi_-(x)$. In terms of the coefficients (b_+, b_-), (a_+, a_-), the bilinear form (2.34) is given by the matrix

$$\begin{pmatrix} 0 & W(\tilde\psi_+, \psi_-) \\ W(\tilde\psi_-, \psi_+) & 0 \end{pmatrix},$$

since

$$W(\tilde\psi_\pm, \psi_\pm) = \lim_{x\to\pm\infty} W(\tilde\psi_\pm, \psi_\pm; x) = 0\,. \tag{2.36}$$

Hence $W(\tilde\psi_-, \psi_+)$ is regular.

Remark. The bilinear used in (2.12) is

$$B(\tilde\psi, \psi) = \int_0^1 dx\,\tilde\psi(x)\psi(x)\,.$$

Non-degeneracy of (2.33) amounts to

$$\int_0^1 dx\,\psi_-(x)\psi_+(x) \neq 0\,,$$

where $\psi_- \in \tilde S^-_{(z,s)} = S^-_{(z,s)}$, $\psi_+ \in S^+_{(z,s)}$ are unique up to non-zero multiples.

2.3. Proofs. Here we prove Theorems 1 and 2, and Lemma 3.

First however we should dwell on a little point of precision about the definition of the current: the current, informally given as

$$I = \mathrm{i}[H, \theta(x)] = -\mathrm{i}\{\frac{d}{dx}, \delta(x)\}\,, \tag{2.37}$$

is not a well-defined operator on Hilbert space. (We suppressed s from the notation and set $x_0 = 0$.) Instead, it should be understood as the map $D(H) \to D(H)^*$,

$$I = \mathrm{i}(\gamma_1^*\gamma_0 - \gamma_0^*\gamma_1)\,,$$

where $\gamma_0, \gamma_1 : D(H) \to \mathbb{C}^n$ with $\gamma_0\psi = \psi(0)$, $\gamma_1\psi = \psi'(0)$. Then (2.37) is replaced by

$$\mathrm{i}[R(z), \theta(x)] = -R(z)IR(z)\,, \tag{2.38}$$

which can be verified first as a quadratic form. This operator is of trace class because $(p^2+1)^{-1}\gamma_i^*\gamma_j(p^2+1)^{-1}$ is.

Given an operator $K : D(H)^* \to D(H)$ one may, pretending cyclicity, take

$$\mathrm{Tr}(IK) := \mathrm{i}\,\mathrm{tr}(\gamma_0 K\gamma_1^* - \gamma_1 K\gamma_0^*)$$

as a definition. In fact, this is the trace of the finite rank operator IK on the Banach space $D(H)^*$, see e.g. [**57**], Eq. (10.2). It yields

$$\mathrm{Tr}(IK) := \mathrm{tr}(-\mathrm{i}\partial_1 K(0,0) + \mathrm{i}\partial_2 K(0,0))\,, \tag{2.39}$$

where $K(x,y)$ is the integral kernel of K and ∂_1 and ∂_2 indicate a derivative w.r.t. the first, resp. second argument. As a further motivation we note that expectation values of the current are naturally written as $\mathrm{Tr}(P_0IP_0)$ and $\mathrm{Tr}(P_0IP_1 + P_1IP_0)$ in zeroth and first order in ω. Then

$$\mathrm{Tr}(P_0IP_0) = \mathrm{i}\,\mathrm{Tr}\big(P_0(\gamma_1^*\gamma_0 - \gamma_0^*\gamma_1)P_0\big) = \mathrm{i}\,\mathrm{tr}(\gamma_0 P_0\gamma_1^* - \gamma_1 P_0\gamma_0^*)\,, \tag{2.40}$$

where cyclicity is now justified since $P_0\gamma_i^*\gamma_j P_0$ is trace class; also, $P_0^2 = P_0$ was used. Similarly,

$$\mathrm{Tr}(P_0IP_1 + P_1IP_0) = \mathrm{i}\,\mathrm{tr}(\gamma_0 P_1\gamma_1^* - \gamma_1 P_1\gamma_0^*)\,,$$

by $P_0P_1 + P_1P_0 = P_1$.

We can now proceed to the proof of Theorem 1

Proof of Theorem 1. The projection P_0 has the integral representation $P_0 = -(2\pi\mathrm{i})^{-1}\oint_\gamma R(z)\,dz$. Since $\oint_\gamma R(z)^2\,dz = 0$ we may replace $R(z)$ therein by $R(z) - R(z)^2H = -zR(z)^2$:

$$P_0 = \frac{1}{2\pi\mathrm{i}}\oint_\gamma zR(z)^2\,dz\,.$$

We then have, by (2.40, 2.38),

$$\begin{aligned}\mathrm{Tr}(P_0IP_0) &= \frac{1}{2\pi}\oint_\gamma z\,\mathrm{tr}(\gamma_0 R(z)^2\gamma_1^* - \gamma_1 R(z)^2\gamma_0^*)\,dz \\ &= \frac{1}{2\pi}\oint_\gamma z\,\mathrm{Tr}\big(R(z)(\gamma_1^*\gamma_0 - \gamma_0^*\gamma_1)R(z)\big)\,dz = -\frac{1}{2\pi}\oint_\gamma z\,\mathrm{Tr}([R(z),\theta(x)])\,dz\,, \end{aligned} \tag{2.41}$$

and, by $zR(z) = HR(z) - 1$, also $\mathrm{Tr}(P_0IP_0) = \mathrm{i}\,\mathrm{Tr}[HP_0,\theta]$. As the stationarity of P_0 suggests, the current is independent of x_0. In fact, upon replacing $\theta(x)$ by $\tilde\theta(x) = \theta(x - x_0) - \theta(x)$ both terms in $\mathrm{Tr}((HP_0)\tilde\theta - \tilde\theta(HP_0))$ are separately trace class, whence the trace vanishes ([**57**], Corollary 3.8). We next turn to (2.41). The commutator $A = [R(z),\theta(x)]$ has integral kernel $A(x,y) = G(x,y)(\theta(y) - \theta(x))$, where $G(x,x') = R(z)(x,x')$ is the Green function. Since $\mathrm{Tr}(P_0IP_0)$ is independent of x_0, we may average over it instead of setting it to 0, thus effectively smoothing θ. We will see in (2.43, 2.45) below that $G(x,y)$ is continuous. Thus $A(x,x) = 0$, implying $\mathrm{Tr}(P_0IP_0) = 0$. The conclusion may be reached without smoothing by resorting to Brislawn's theorem ([**57**], Theorem A.2), according to which $\mathrm{Tr}\,A = \int dx\,\tilde A(x,x)$, where $\tilde A(x,y)$ is the Lebesgue value of $A(x,y)$. Here, $\tilde A(x,x) = 0$. ■

Theorem 2 is proven expressing the Green function in term of the $\psi_\pm$, and then calculating the trace with (2.39) on one side; and finding expressions for $\partial_z\psi_\pm$ and inserting them it in (2.25) on the other.

Proof of Theorem 2. By applying (2.39) to $K = R(z,s)\dot R(z,s)$ in (2.6, 2.26) we obtain for the transported charge

$$\langle Q_T\rangle = \frac{\mathrm{i}}{2\pi}\oint ds\oint_\gamma dz\int dx\ \mathrm{tr}\big(\partial_1 G(0,x)\dot G(x,0) - G(0,x)\partial_2\dot G(x,0)\big)\,. \tag{2.42}$$

We claim that the Green function can be expressed as

$$G(x,x') = -\theta(x-x')\psi_+(x)\tilde\psi_-(x') - \theta(x'-x)\psi_-(x)\tilde\psi_+(x')\,, \tag{2.43}$$

where we complemented the locally smooth choice of $\psi_+ \in S^+_{(z,s)}$, $\tilde\psi_- \in \tilde S^-_{(z,s)}$ satisfying (2.24) by that of a pair $\tilde\psi_+ \in \tilde S^+_{(z,s)}$, $\psi_- \in S^-_{(z,s)}$ with

$$W(\tilde\psi_+,\psi_-) = -1\,. \tag{2.44}$$

Indeed, because of (2.24, 2.44) and of (2.36) the general column solution (2.35) has coefficients

$$a_\pm = \pm W(\tilde\psi_\mp,\varphi) = \pm\tilde\psi_\mp(y)\varphi'(y) \mp \tilde\psi'_\pm(y)\varphi(y)\,.$$

By inserting this in (2.35) and in its derivative w.r.t. x, and by setting $y = x$, we conclude from the arbitrariness of $\varphi(x)$ and $\varphi'(x)$ that

$$\begin{aligned}\psi_+(x)\tilde{\psi}_-(x) - \psi_-(x)\tilde{\psi}_+(x) &= 0\,,\\ \psi_+(x)\tilde{\psi}'_-(x) - \psi_-(x)\tilde{\psi}'_+(x) &= -1\,,\\ \psi'_+(x)\tilde{\psi}_-(x) - \psi'_-(x)\tilde{\psi}_+(x) &= 1\,.\end{aligned} \tag{2.45}$$

By means of these relations one verifies that G, as given by the r.h.s. of (2.43), satisfies

$$\Big(-\frac{d^2}{dx^2} + V(x) - z\Big)G(x,x') = \delta(x-x')1\,;$$

together with $G(x,x') \to 0$, $(|x| \to \infty)$, which exhibits it as the Green function. We then apply (2.43) in Eq. (2.42): For $x \geq 0$ the integrand is

$$\begin{aligned}&\mathrm{tr}\big(\partial_1 G(0,x)\dot{G}(x,0) - G(0,x)\partial_2\dot{G}(x,0)\big) = \\ &\mathrm{tr}\big(\psi'_-(0)\tilde{\psi}_+(x)(\dot{\psi}_+(x)\tilde{\psi}_-(0) + \psi_+(x)\dot{\tilde{\psi}}_-(0)) - \psi_-(0)\tilde{\psi}_+(x)(\dot{\psi}_+(x)\tilde{\psi}'_-(0) + \psi_+(x)\dot{\tilde{\psi}}'_-(0))\big)\\ &\qquad = \mathrm{tr}\big(W(\dot{\tilde{\psi}}_-,\psi_-)\,\tilde{\psi}_+(x)\psi_+(x)\big)\,,\end{aligned}$$

where we used cyclicity of the trace and (2.36). Here and henceforth the Wronskian is evaluated at $x = 0$, unless otherwise stated. Together with a similar computation for $x \leq 0$ we obtain

$$\langle Q_T\rangle = \frac{\mathrm{i}}{2\pi}\oint ds \oint_\gamma dz\ \mathrm{tr}\big(W(\dot{\tilde{\psi}}_-,\psi_-)\int_0^\infty dx\,\tilde{\psi}_+(x)\psi_+(x) + W(\dot{\tilde{\psi}}_+,\psi_+)\int_{-\infty}^0 dx\,\tilde{\psi}_-(x)\psi_-(x)\big)\,. \tag{2.46}$$

We maintain that the same expression is obtained from a computation of C, the r.h.s. of (2.25). That calls for one of $\partial\psi_+/\partial z$, $\partial\tilde{\psi}_-/\partial z$. Differentiating (2.18) w.r.t. z we obtain

$$\Big(-\frac{d^2}{dx^2} + V(x,s) - z\Big)\frac{\partial\psi_+}{\partial z} = \psi_+\,,$$

whose general solution with $\partial\psi_+/\partial z \to 0$, $(x \to \infty)$ is

$$\frac{\partial\psi_+}{\partial z}(x) = \psi_+(x)F_+(x) - \psi_-(x)\int_x^\infty \tilde{\psi}_+(x')\psi_+(x')dx'\,, \tag{2.47}$$

where $F'_+(x) = dF_+/dx = -\tilde{\psi}_-(x)\psi_+(x)$. Hence F_+ is determined up to an additive constant, which reflects the gauge freedom (2.23) of ψ_+. Eq. (2.47) is verified by twice differentiating it w.r.t. x, the first derivative being

$$\frac{\partial\psi'_+}{\partial z}(x) = \psi'_+(x)F_+(x) - \psi'_-(x)\int_x^\infty \tilde{\psi}_+(x')\psi_+(x')dx'\,,$$

by using (2.45). In the same way we find

$$\frac{\partial\tilde{\psi}_-}{\partial z}(x) = F_-(x)\tilde{\psi}_-(x) - \Big(\int_{-\infty}^x \tilde{\psi}_-(x')\psi_-(x')dx'\Big)\tilde{\psi}_+(x)\,,$$

with $F'_- = -F'_+$. The arbitrariness of $F_\pm$ is constrained by (2.24), which implies

$$F_+ + F_- = 0\,. \tag{2.48}$$

This is seen by differentiating the constraint w.r.t. z and by using

$$W(\tilde\psi_-, \frac{\partial\psi_+}{\partial z}; x) = W(\tilde\psi_-, \psi_+; x)F_+(x) - W(\tilde\psi_-, \psi_-; x)\int_x^\infty \tilde\psi_+(x)\psi_+(x)\,dx = F_+(x)\,,$$
$$W(\frac{\partial\tilde\psi_-}{\partial z}, \psi_+; x) = F_-(x)\,.$$

Similarly, differentiating the constraint w.r.t. s yields

$$W(\dot{\tilde\psi}_-, \psi_+; x) + W(\tilde\psi_-, \dot\psi_+; x) = 0\,. \tag{2.49}$$

We are now in position to compute C and in particular

$$\begin{aligned}
W(\frac{\partial\tilde\psi_-}{\partial s}, \frac{\partial\psi_+}{\partial z}) =& \dot{\tilde\psi}_-(0)\big(\psi'_+(0)F_+(0) - \psi'_-(0)\int_0^\infty \tilde\psi_+(x)\psi_+(x)\,dx\big)\\
&- \dot{\tilde\psi}'_-(0)\big(\psi_+(0)F_+(0) - \psi_-(0)\int_0^\infty \tilde\psi_+(x)\psi_+(x)\,dx\big)\\
=& W(\dot{\tilde\psi}_-, \psi_+)F_+(0) - W(\dot{\tilde\psi}_-, \psi_-)\int_0^\infty \tilde\psi_+(x)\psi_+(x)\,dx\,,\\
W(\frac{\partial\tilde\psi_-}{\partial z}, \frac{\partial\psi_+}{\partial s}) =& F_-(0)W(\tilde\psi_-, \dot\psi_+) - \Big(\int_{-\infty}^0 \tilde\psi_-(x)\psi_-(x)\,dx\Big)W(\tilde\psi_+, \dot\psi_+)\,,
\end{aligned}$$

Taking the trace of difference of the two expressions, the first terms on the r.h.s. cancel because of (2.48, 2.49). The result is that C agrees with the r.h.s. of (2.46). ■

We conclude this chapter with the proof of Lemma 3.

Proof of lemma 3. In Eq. (2.3) $P_1(s)$ is uniquely determined [**44**] by the conditions

$$\begin{aligned}
\mathrm{i}\dot P_0(s) &= [H, P_1(s)]\,,\\
P_0(s)P_1(s) + P_1(s)P_0(s) &= P_1(s)\,,
\end{aligned} \tag{2.50}$$

which are obtained by differentiating the expansion w.r.t. s, respectively from the fact that it represents a projection. We omit s from the notation in the rest of the proof. Eq. (2.26) satisfies the first condition because of

$$[H, P_1] = -\frac{1}{2\pi}\oint_\gamma [H - z, R(z)\dot R(z)]dz = -\frac{1}{2\pi}\oint_\gamma (\dot R(z) + R(z)^2\dot H)dz\,,$$

where we expanded the commutator and used $\dot R = -R\dot H R$. The second contribution vanishes and the first yields the claim by $P_0 = -(2\pi\mathrm{i})^{-1}\oint_\gamma R(z)\,dz$. The second condition (2.50) is equivalent to $P_0P_1P_0 = 0$, $(1-P_0)P_1(1-P_0) = 0$, which are satisfied, too:

we rewrite $\dot{R}$ as before and use the spectral representation $P = \int_I dP_\lambda$ to compute

$$P_0 P_1 P_0 = \int_I \int_I (dP_\lambda) \dot{H} (dP_\mu) \oint_\gamma dz \frac{1}{(\lambda - z)^2 (\mu - z)} = 0\,;$$

similarly, $(1 - P_0) P_1 (1 - P_0) = 0$. □

Alternatively, one can directly verify the equality between (2.26) and (2.4) by a longer calculation.

CHAPTER 3

The scattering approach to pumping

In this second chapter we present the scattering approach to quantum pumping. In the scattering approach the pump is modelled as a time-dependent scatterer connected to several leads. Each lead may have several channels. Each channel is modelled as a semi-infinite, one dimensional, single mode ideal wire. As a consequence the particles in the channels move freely. The interaction with the scatterer happens on a time scale τ, the typical dwell time near the scatterer. The theory we are going to present considers non-interacting fermions, all with dispersion relation $\epsilon(k)$, with the assumption that the state of the incoming electrons is described by the density matrix ρ common to all channels $\rho(E) = (1 + \mathrm{e}^{\beta(E-\mu)})^{-1}$, with Fermi energy μ and temperature $T = \beta^{-1}$. The theory is mostly valid for general dispersion relations, but for the sake of concreteness let us stick to $\epsilon(k) = k^2$.

The time dependence of the scatterer is considered to be adiabatic, which means that the characteristic frequency of the scatterer ω is small compared to the inverse of the dwell time near the scatterer $\omega \ll \tau^{-1}$.

The interest focuses on the transport of particles from one channel to another. The first quantity one would want to know, in order to characterize the transport of particles, is the expectation value of the net charge transport to a given channel, either in a cycle or even locally in time. The work of Büttiker, Prêtre and Thomas [**22, 21**] (see also [**42, 43**]) addresses this question in the context of linear response theory and provides with a formula (we will call this formula the BPT formula) that allows to calculate the expectation value of the instantaneous current from time-independent scattering data. The BPT formula may be rewritten as a surface integral, as first noted by Brouwer [**16**].

Other quantity of interest to characterize charge transport are energy dissipation, noise currents and entropy currents [**19, 28**]. They all depend, together with the current, on a single quantity, the matrix of energy shift $\mathcal{E}$. The matrix of energy shift is constructed from the scattering matrix and its time derivative. It is the first order (in ω) approximation of the operator of energy shift, which relates the state of incoming particle to the outgoing state.

The expected current is of order ω^1 and involves the diagonal elements of the matrix of energy shift. Energy dissipation, noise and entropy currents all depend quadratically on the off-diagonal term of $\mathcal{E}$, and appear at order ω^2. One could hope that this is the beginning of a power series expansion in ω, fully characterizing charge transport through

time-independent scattering data. This is however impossible, as we will present examples of processes with identical scattering matrices, but whose charge and energy transport agree only to leading order.

Adiabatic scattering is characterized by the fact that an incoming particle interacts with the scatterer on a time scale which is much shorter then the time scale over which the scatterer varies. The particle sees a quasi-static scatterer, and the leading order of scattering is computed with time-independent quantum mechanics, by pretending that the Hamiltonian has ever been, and will always be, $H(t)$, the one in action at the time t where the particle reaches the scatterer [**20, 39**]. This produces the frozen scattering matrix S_f, which is the ω^0 approximation of the full dynamical scattering matrix S_d. Scattering theory is a comparison of dynamics: the evolution generated by the (possibly non-autonomous) Hamiltonian H is compared to the one generated by H_0, a time-independent Hamiltonian, called the free Hamiltonian. As time-independent scattering conserves energy (as defined by H_0), the frozen scattering matrix commutes with H_0, and S_f possesses the direct decomposition $S_f = \int^{\oplus} dE S(E,t)$. $S(E,t)$ is the on-shell frozen S matrix, and if H_0 is chosen correctly it corresponds to the familiar physical definition in term of transmission and reflection coefficients.

At order ω^0 there is no transport: as the incoming densities are all equal, the unitarity of $S(E,t)$ implies that the outgoing densities will be the same as the incoming ones. At order ω^1, however, transport is produced by an interesting interference phenomenon: the uncertainty principle implies that a wave packed with a well defined energy cannot have a well defined scattering time. The tail of the wave packet sees therefore a slightly different scatterer with respect to the one seen by the head of the wave packet. This differential scattering causes the outgoing density to differ slightly from the ingoing one. The spread in time of the wave packet is caused by the uncertainty principle and has nothing to do with the dwell time near the scatterer. As the uncertainty $\delta E \delta t$ is of order ω^1, the leading order of the transport will be ω^1, and one may hope to obtain it using semiclassical methods. This is indeed possible, and we will present the derivation of the formulae for charge transport, dissipation and entropy/noise currents in this form, following closely [**10**].

We now introduce the promised formulae for the mentioned quantities. They all depend on the matrix of energy shift [**39**]

$$\mathcal{E}(E,t) = \mathrm{i}\dot{S}(E,t)S(E,t)^*\,,$$

(with the dot denoting derivative with respect to time) which is dual to the Wigner time delay [**69**]

$$\mathcal{T} = -\mathrm{i}S(E,t)'S(E,t)^*\,,$$

where $'$ denotes derivative with respect to energy. Their commutator

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

has a geometrical meaning as curvature in the energy-time plane, and in a semiclassical setting is deeply related with the arousal of currents, as explained in Appendix 2.

The expectation value of the current to j-th channel, $\langle \dot{Q} \rangle_j$ is given by the BPT formula

$$\langle \dot{Q} \rangle_j(t) = -\frac{1}{2\pi} \int_0^\infty dE \rho'(E-\mu) \mathcal{E}_{jj}(E,t)\,. \tag{3.1}$$

The current depends on the diagonal elements of the matrix of energy shift. At $T = 0$, the occupation density is a step function, and the current is determined by the matrix of energy shift at the Fermi energy alone. Two facts about (3.1) need to be mentioned: the first is that the current $\langle \dot{Q} \rangle_j$, which is a first order quantity, is accurately computed in terms of the frozen scattering data, which are a ω^0 approximation of the dynamical ones. The second is that the formula is valid for all temperatures, down to $T = 0$, where the energy scale T^{-1} is large with respect to the adiabatic energy scale ω^{-1}.

The matrix of energy shift also determines the dissipation. Dissipation is caused by the fact that as the electrons are dumped into the reservoirs, some energy is lost forever. It is therefore natural to define dissipation in channel j as the difference between the energy flux $\langle \dot{E} \rangle_j$ into the channel and the part of it that may be recovered by reclaiming the particles $\mu \langle \dot{Q} \rangle_j$. The dissipation may be computed, at $T = 0$ and to lower order, by the formula

$$\langle \dot{E} \rangle_j - \mu \langle \dot{Q} \rangle_j = \frac{1}{4\pi} (\mathcal{E}^2)_{jj}(\mu, t) \geq 0\,. \tag{3.2}$$

Dissipation is therefore a quantity of order ω^2. This is surprising as it is the difference of two first order quantities. This is related to the fact that in each quantum channel one has the bound [**8**]

$$\langle \dot{E} \rangle_j - \mu \langle \dot{Q} \rangle_j \geq \pi \langle \dot{Q} \rangle_j^2\,. \tag{3.3}$$

Pumps saturating the bound (3.3) are called optimal (with respect to channel j). Optimal quantum pumps produce a quantized charge transport, by which we mean that charge transport over a cycle not only has an integer expectation value, but also a vanishing variance.

The entropy and noise currents are defined as the difference between ingoing and outgoing currents:

$$\dot{s}_j(t, \mu, T) = \dot{s}(\rho_{\mathrm{out},j}) - \dot{s}(\rho_j) \tag{3.4}$$

$$\dot{s}(\rho) = \frac{1}{2\pi} \int dE (h \circ \rho)(E,t)\,, \tag{3.5}$$

where [**18, 19, 28**]

$$h(x) = \begin{cases} -x\log x - (1-x)\log(1-x) & \text{entropy} \\ x(1-x) & \text{noise} \end{cases} \tag{3.6}$$

The noise and entropy current at finite temperatures (in the regime $\omega \ll T \ll \sqrt{\omega/\tau}$) are given by

$$\dot{s}_j(t,\mu,T) = \frac{\beta}{2\pi k}\Delta\mathcal{E}_j^2(\mu,t) \geq 0\,, \qquad k = \begin{cases} 2 & \text{entropy} \\ 6 & \text{noise} \end{cases}\,, \tag{3.7}$$

where

$$\Delta\mathcal{E}_j^2 = (\mathcal{E}^2)_{jj} - (\mathcal{E}_{jj})^2 = \sum_{j\neq k} |\mathcal{E}_{jk}|^2\,. \tag{3.8}$$

The starting point for the derivation of all these results is the equation

$$\rho_{\text{out}}(H_0) = \rho(H_0 - \mathcal{E}_d) \tag{3.9}$$

relating the outgoing to the incoming density. $\mathcal{E}_d$ is the (dynamical) operator of energy shift, defined as

$$\mathcal{E}_d = \mathrm{i}\dot{S}_d S_d^*$$

The equality (3.9) is exact. In the adiabatic limit, the operator of energy shift acting on states with an approximate time of passage t may be approximated by the matrix of energy shift evaluated at time t. More precisely, if one describes the adiabatic limit as a semiclassical limit using Weyl calculus, the matrix of energy shift is found to be the principal symbol corresponding to the operator of energy shift.

The BPT formula and the formula for the dissipation hold all the way down to $T = 0$. This is surprising because one could expect response formulae at $T = 0$ to display memory effects, due to the slow decay of correlations. This is not the case for charge transport and dissipation, which are described by formulae which are local in time. It is however the case for the entropy and noise currents: there is no local description of these quantities holding at $T = 0$. The reason for this different behaviour is the fact that charge transport and dissipation, as described by (3.1) resp. (3.2), depend linearly in the density ρ. Entropy and noise current have a nonlinear dependence on ρ, whence their sensitivity to slow decay of correlations at $T = 0$.

Instead of looking for a description of charge transport which is local in time, one could ask about the statistics of transport over a complete cycle of the pump. This is the content of the theory of full counting statistics [**36, 35, 29, 5**]. It allows the computation of all the moments of charge transport over a cycle; this description is valid at $T = 0$ for all moments, but it determines transport over a complete cycle in terms of the entire history of the pump. We will give a short description of results of the theory of full counting statistics concerning the quantities introduced above at the end of this chapter.

A remarkable fact about the scattering approach to quantum pumping is that it produces a geometrical description of transport. The geometrical significance of the BPT formula is related to Berry's phase, and the rewriting of it as a surface integral [**16, 72**] may be interpreted as curvature and is formally related to the adiabatic curvature. Also the dissipation may be understood in geometrical terms, as the notion of optimality. The quantization of charge transport for optimal pumps is very clearly explained, as for such pumps charge transport is a winding number; this quantization is however not stable: a small perturbation of the cycle in the space of scattering matrices is sufficient to drive the pump away from optimality. In this context it will be clear that optimal pumps transport a quantized number of particles not only in the sense that the expectation value is an integer: the variance of charge transport over a cycle vanishes for such pumps, and every realization of the cycle transport the same number of particles. Although the scattering approach to pumping has a very interesting and rich geometry, the topological content is trivial.

The chapter is organized as follows: in Section 1 we will recall some basic elements of scattering theory and then derive the basic relation (3.9) between incoming and outgoing density. In Section 2 we report various derivations of the formulae (3.1), (3.2) and (3.4), starting from an elementary derivation of BPT in the two channel case and then presenting the semiclassical approach to adiabatic quantum transport. We will conclude the section reporting on a rigorous mathematical proof of the BPT equation (3.1). In Section 3 we will present the geometrical content of adiabatic quantum pumping. Some examples will follow in Section 4. We will conclude with a brief description of the results of the theory of full quantum statistics, mainly for the sake of comparison, in Section 5.

1. The operator of energy shift

In this section we quickly recall some basic elements in scattering theory with the aim of introducing and describing the operator of energy shift and his frozen analogon, the matrix of energy shift. In particular we derive the equality (3.9) relating the outgoing density matrix to the incoming one through the operator of energy shift. This equality will be the starting point of the analysis of adiabatic quantum transport given in the next section.

1.1. The dynamical and the frozen S matrices. Scattering theory is a comparison of dynamics: the actual dynamics generated from $H(t) = H_0 + V(t)$ is compared to the dynamics generated by the reference time-independent Hamiltonian H_0 (often called the free Hamiltonian).

Let $U(t_2, t_1)$ be the non-autonomous evolution from t_1 to t_2 generated by $H(t)$ and

$U_0(t_2,t_1) = \mathrm{e}^{-\mathrm{i}(t_2-t_1)H_0}$ be the free evolution, we assume the existence of the wave operators (for conditions ensuring this see for instance [**70, 50**]), defined as the (strong) limits

$$\Omega_\pm(t_0,H,H_0) := s - \lim_{t_1\to\pm\infty} U(t_0,t_1)U_0(t_1-t_0)\,. \tag{3.10}$$

The existence of the limit and the equation of motion imply that the dependence of the wave operators on the base point t_0 satisfies the differential equation:

$$\mathrm{i}\partial_{t_0}\Omega_\pm(t_0,H,H_0) = H(t)\Omega_\pm(t_0,H,H_0) - \Omega_\pm(t_0,H,H_0)H_0\,. \tag{3.11}$$

If the Hamiltonian H is time-independent, and the evolution U is therefore autonomous, $\Omega_\pm(t_0,H,H_0)$ is independent on the base point, as in this case the limit $t_1\to\pm\infty$ is equivalent to the limit $t_1 - t\to\pm\infty$. The frozen wave operators, comparing the frozen dynamics $U_f^{(t)}(t_2-t_1) = \mathrm{e}^{-\mathrm{i}(t_2-t_1)H(t)}$ to the free dynamics U_0, have therefore no dependence on the base point t_0, and the dependence on t is purely parametric. We denote them by $\Omega_{f\pm}(H(t),H_0)$. It is now a consequence of (3.11) that the frozen wave operators intertwine the frozen and the free dynamics:

$$H(t)\Omega_{f\pm}(H(t),H_0) = \Omega_{f\pm}(H(t),H_0)H_0\,. \tag{3.12}$$

The scattering matrices map incoming states (denoted by their asymptotically free past trajectories) to outgoing states (denoted by their asymptotically free future trajectories). The dynamical and the frozen scattering matrices are defined as

$$\begin{aligned} S_d(t,H,H_0) &= \Omega_+^*(t,H,H_0)\Omega_-(t,H,H_0)\\ S_f(H(t),H_0) &= \Omega_{f+}^*(H(t),H_0)\Omega_{f-}(H(t),H_0)\,. \end{aligned}$$

time-independent scattering conserves energy, whereas time-dependent does not. In the time-independent case this is expressed as the fact that the scattering matrix commutes with the free (not the full) Hamiltonian, as seen by (3.12). It follows for the frozen scattering matrix:

$$S_f(H(t),H_0)\mathrm{e}^{-\mathrm{i}t'H_0} = \mathrm{e}^{-\mathrm{i}t'H_0}S_f(H(t),H_0)\,. \tag{3.13}$$

This equality admits the following interpretation: if the scattering is time-independent a state $|\psi\rangle$ and the time translated state $\mathrm{e}^{-\mathrm{i}t'H(t)}|\psi\rangle$ both see the same scatterer.

This is no longer true in the time-dependent case, and the dynamical S matrix assumes a time dependence

$$S_d(t)\mathrm{e}^{-\mathrm{i}tH_0} = \mathrm{e}^{-\mathrm{i}tH_0}S_d(0)\,. \tag{3.14}$$

This equality follows from $U(t,t')\Omega_\pm(t') = \Omega_\pm(t)\mathrm{e}^{-\mathrm{i}(t-t')H_0}$, which in turn is a trivial consequence of (3.10). As all the dynamical S matrices are related by conjugation, anyone of them is unitarily equivalent to any other. To pick one amounts to pick a reference point in time. We shall henceforth write S_d for $S_d(0)$.

We define now the frozen on-shell scattering matrix: let $|E, j\rangle$ be the (improper) state in the j-th channel with energy E, the fact that frozen scattering is energy conserving implies

$$\langle E', j'|S_f(H(t), H_0)|E, j\rangle = \delta(E - E')S_{jj'}(E, t)\,. \tag{3.15}$$

$S_{jj'}(E, t)$ is the frozen on-shell scattering matrix.

1.2. The energy shift. Taking the time derivative of (3.13) one obtains the equation of motion

$$\mathrm{i}\dot{S}_d(t) = [H_0, S_d(t)]\,. \tag{3.16}$$

If $S_d(t)$ is unitary, what we assume from now on (S_d is unitary as a map between the spaces of in and out states, which may differ because particles may be trapped or released by the pump), (3.16) may be rewritten as

$$\mathrm{i}\dot{S}_d(t)S_d(t)^* = H_0 - S_d(t)H_0S_d(t)^*\,. \tag{3.17}$$

If H_0 is the operator corresponding with the asymptotic observable of outgoing energy, then $S_d(t)H_0S_d(t)^*$ correspond to the incoming energy, and (3.17) motivates calling

$$\mathcal{E}_d(t) := \mathrm{i}\dot{S}_d(t)S_d(t)^*$$

the operator of energy shift. The assumed unitarity of $S_d(t)$ is reflected in the self-adjointeness of the energy shift.

The time dependence of the energy shift is read from (3.17):

$$\mathcal{E}_d(t) = \mathrm{e}^{\mathrm{i}H_0t}\mathcal{E}_d(0)\mathrm{e}^{-\mathrm{i}H_0t}\,.$$

If the incoming state is described by the density matrix $\rho_{\mathrm{in}}(H_0)$, then the outgoing state is $\rho_{\mathrm{out}} = S_d\rho_{\mathrm{in}}(H_0)S_d^*$. The application of functional calculus to (3.17) (evaluated at $t = 0$), provides the starting point for the analysis of adiabatic transport:

$$\rho_{\mathrm{out}} = \rho_{\mathrm{in}}(H_0 - \mathcal{E}_d)\,. \tag{3.18}$$

This equality is exact, and it does not assume adiabatic time dependence. In the adiabatic limit we can approximate the energy shift acting on states with approximate time of passage t with the matrix of energy shift

$$\mathcal{E}(E, t) = \mathrm{i}\dot{\mathcal{S}}(E, t)\mathcal{S}(E, t)^*\,.$$

2. Derivations

In this section we present some derivations of the formulae (3.1), (3.2) and (3.4) characterizing charge transport. We start by a derivation [**7**] of the BPT formula at $T = 0$ and for the two channel case. The authors called this derivation "pedestrian", as it is obtained describing changes in the scattering matrix by elementary processes, such as translating the scatterer or applying a vector potential, and the BPT formula follows then by simple physical considerations and known facts.

We then pass to the main part of the section, a description of adiabatic quantum transport as a semiclassical limit [**10, 53, 38**]. In fact, as suggested in the introduction of this chapter, the current induced by a slowly changing scatterer is an interference phenomenon caused by the Heisenberg uncertainty relation $\delta E \delta t \approx \omega$, and may be analysed with the help of Weyl calculus (a description of Weyl calculus is given in Appendix A).

The analysis bases on equation (3.17), where in the adiabatic limit the operator of energy shift, acting on states of approximate time of passage t, is approximated by the matrix $S(E, t)$ constructed from time-independent scattering data. In the language of Weyl calculus, $S(E, t)$ is the principal symbol associated to the operator of energy shift. Having proven this assignment it will be possible to derive the formulae describing currents (the BPT formula), dissipation and entropy and noise currents, as stated in the introduction to the chapter.

At the end of this section we will report on a fully rigorous mathematical proof of the BPT formula (3.1).

2.1. Derivation of BPT in the two channel case.

We now report an argument [**7**] that explains the BPT formula in the two channel case and at $T = 0$. This case is special in that changes in the scattering matrix can be described in terms of elementary processes and the charge transport may be understood with the help of simple physical considerations and known facts.

In the two channel case the frozen on shell scattering matrix has the form

$$S(E) = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}(E)\,,$$

and at $T = 0$ the derivative of the density matrix is $-\rho'(E) = \delta(E - \mu)$, so that the BPT formula states

$$2\pi\langle dQ\rangle_1 = \mathrm{i}(\overline{r}'dr' + \overline{t}dt)\,, \qquad 2\pi\langle dQ\rangle_2 = \mathrm{i}(\overline{r}dr + \overline{t}'dt')\,,$$

where the transmission and reflection coefficients are evaluated at the Fermi energy μ.

We observe that every unitary 2×2 matrix can be written in term of the four real parameters $(\theta,\, \alpha,\, \varphi,\, \gamma)$ as

$$S = \mathrm{e}^{\mathrm{i}\gamma} \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha} \cos\theta & \mathrm{e}^{-\mathrm{i}\varphi} \sin\theta \\ \mathrm{e}^{\mathrm{i}\varphi} \sin\theta & \mathrm{e}^{-\mathrm{i}\alpha} \cos\theta \end{pmatrix},$$

where $0 \leq \alpha\,, \varphi \leq 2\pi,\ 0 \leq \gamma \leq \pi,\ 0 \leq \theta \leq \pi/2$. The four parameters, and the changes thereof, admit the following physical interpretation: changes in the parameter α are associated with translations of the scatterer, φ is related with the presence of a vector potential across the pump, the parameter θ determines the conductance of the system, and γ is associated to the number of electrons trapped by the scatterer. The strategy of the argument consists therefore in breaking down the changes in the scattering matrix into elementary physical processes, and to verify that the charge transport they produce is given by the BPT formula, written in terms of the introduced parameters as

$$2\pi \langle dQ \rangle_{1,2} = \mp(\cos^2\theta) d\alpha \pm (\sin^2\theta) d\varphi - d\gamma\,. \tag{3.19}$$

The argument relies on the assumption that the charge transport (to first order in ω) depends only on $S(\mu)$ and, linearly, on $dS(\mu)$ and is therefore not a complete proof. We now proceed to the analysis of the effect of changes of the four parameters.

2.1.1. *Translations of the scatterer.* We begin by the parameter α. As announced changes in α are caused by translations of the scatterer: in fact, if we denote by k_F the momentum associated with the Fermi energy, translating the scatterer a distance dL has the only consequence of adding $2k_F dL$ to the phase of reflected particles, i.e. produces a change

$$r \longrightarrow r\mathrm{e}^{\mathrm{i}2k_F dL} \qquad r' \longrightarrow r'\mathrm{e}^{-\mathrm{i}2k_F dL}\,,$$

leaving t, t' unchanged. Therefore $d\alpha = 2k_F dL$ corresponds to shifting the scatterer.

As the scatterer traverses a region of length dL, it encounters $k_F dL/\pi = d\alpha/2\pi$ electrons. Of those, a fraction $|t|^2 = \sin^2\theta$ will pass through the scatterer (or better the scatterer will pass through them), while a fraction $|r|^2 = \cos^2\theta$ will be pushed forward, producing a charge transport

$$2\pi \langle Q \rangle_{1,2} = \mp(\cos^2\theta) d\alpha\,, \tag{3.20}$$

in accordance with (3.19).

We can get a check of the result above by analysing the special case of an uniform moving scatterer, where we can use a Galilei transformation to obtain the charge transport exactly. The change of coordinates from the lab frame to the moving frame shifts every momentum by an amount $-\dot{L}/2$ (the mass of the electron is two). As a consequence the incoming states in the 1, (resp. 2) channel in the moving frame are filled up to $k_F \mp \dot{L}/2$, whereas the outgoing states are totally filled up to $k = k_F - \dot{L}/2$ and partially

filled with density $|t'(k)|$ (resp. $|r'(k)|$) for energies $k_F - \dot{L}/2 < k \leq k_F$. Transforming back in the lab frame one obtains the occupation density difference $\delta\rho_1$:

$$\delta\rho_1(k^2) = \begin{cases} 0 & \text{if} \quad k < k_F - \dot{L} \\ -|r'(k+\dot{L})|^2 & \text{if} \quad k_F - \dot{L} < k < k_F \\ 0 & \text{if} \quad k > k_F \end{cases}$$

This is, to first order in $\dot{L}$

$$\delta\rho_1 = -2k_F\dot{L}|r'(k_F)|^2\delta(E-\mu)\,,$$

which implies for the charge transport

$$\langle\dot{Q}\rangle_1 = \frac{1}{2\pi}\int_0^\infty dE\delta\rho_1(E) = -2k_F\dot{L}|r'(k_F)|^2\,,$$

in agreement with (3.20).

2.1.2. *The battery.* We now discuss changes in the parameter φ. These are associated with the presence of a vector potential A with $-\int A = \varphi$. In fact a vector potential induces a phase shift across the scatterer and changes the transmission t (resp. t') by multiplication with $\mathrm{e}^{\pm\mathrm{i}\int A}$

$$t \longrightarrow t\mathrm{e}^{\mathrm{i}\int A} \qquad t' \longrightarrow t'\mathrm{e}^{-\mathrm{i}\int A}\,,$$

while leaving the reflection coefficients unchanged. A change in the vector potential A induces an EMF of strength $-\int \dot{A} = -\dot{\phi}$, this in turn produces a current which is equal to the EMF multiplied with the Landauer conductance of the scatterer $|t|^2/2\pi$:

$$2\pi\langle\dot{Q}\rangle_{1,2} = \pm(\sin^2\theta)d\varphi\,, \tag{3.21}$$

in accordance with (3.19).

As an illustration consider now the case of a time-independent voltage drop, a battery. In a gauge where the battery is represented by a scalar potential, the pump is represented by a time-independent scattering problem, with the voltage having slightly different asymptotes at $\pm\infty$. If the battery is placed to the left of the scatterer, the incoming states in channel 1 (resp. 2) will be occupied up to $E = \mu - \dot{\varphi}$ (resp. $E = \mu$). The difference in the occupation density between in and out states in channel 2 is then

$$\delta\rho_2(E) = \begin{cases} 0 & \text{if} \quad E < \mu \\ -|t(E)|^2 & \text{if} \quad \mu < E < \mu + \dot{\varphi} \\ 0 & \text{if} \quad E < \mu + \dot{\varphi} \end{cases}$$

If the battery is placed to the right of the scatterer one finds:

$$\delta\rho_2(E) = \begin{cases} 0 & \text{if} \quad E < \mu \\ -|t(E+\dot{\varphi})|^2 & \text{if} \quad \mu < E < \mu + \dot{\varphi} \\ 0 & \text{if} \quad E < \mu + \dot{\varphi} \end{cases}$$

Both cases are analogous in leading order, where $\delta\rho_2(E) = -\dot\varphi|t(\mu)|^2\delta(E-\mu)$, and the current is

$$\langle\dot Q\rangle_2 = \frac{1}{2\pi}\int_0^\infty dE\delta\rho_1(E) = -\dot\varphi|t(\mu)|^2$$

as predicted by (3.21).

The charge transport at first order in $\dot\varphi$ is insensitive to weather the battery is placed to the right or the left of the scatterer. This is no longer true at $O(\dot\varphi^2)$. The frozen scattering matrix, however, does not capture the difference between the two situations. For this reason it is impossible to find a formula for the charge transport, accurate to order $O(\omega^2)$, depending only on time-independent scattering data.

2.1.3. *The variable gamma.* The scattering matrix depends on the choice of two fiducial points, defining the border between the scatterer and the two channels. Moving each one of these two points a distance dL out results on one hand in the forfeiting of $k_F dL/\pi$ electrons from the channels in favour of the scatterer; on the other hand the scattering matrix acquires an overall phase:

$$S(k_F) \longrightarrow \mathrm{e}^{2\mathrm{i}k_F dL}\,,$$

meaning $d\gamma = 2k_F dL$. The charge transport is therefore, in accord with (3.19)

$$2\pi\langle Q\rangle_{1,2} = -d\gamma\,.$$

It follows that changing γ is equivalent to having the pump swallow electrons from the reservoirs.

This result still holds for arbitrary changes dS for the sum $\langle dQ\rangle_1 + \langle dQ\rangle_2$: this follows from a fact in scattering theory, known as Friedel sum rule [**26**] or Birman-Krein formula [**70**], which states that the number of states with energy $E < \mu$ associated with the scatterer is $(2\pi\mathrm{i})^{-1}\log\det S(\mu)$, with the consequence

$$2\pi(\langle dQ\rangle_1 + \langle dQ\rangle_2) = \mathrm{i}d\log\det S(\mu) = -2d\gamma\,.$$

2.1.4. *The ineffective variable θ.* Till now we have seen that the BPT formula (3.19) reproduces correctly the transport of charge caused by variations of the parameters α, φ and γ, and the sum $\langle Q\rangle_1 + \langle Q\rangle_2$ for general variations of the scattering matrix $S(\mu)$. To conclude the derivation it is therefore sufficient to show that the difference $\langle Q\rangle_1 - \langle Q\rangle_2$ vanishes for changes in the parameter θ, with α, φ and γ kept fixed, as described by (3.1).

To show this we first observe that we can limit our analysis to scatterers with $\alpha = \varphi = 0$, as translating the scatterer a fixed distance, and adding a fixed vector potential we can obtain this.

We compare then the scatterer with his mirror image, i.e. a scatterer obtained from the first by exchanging left and right. As θ and γ are invariant under reflection (whereas

α and φ are odd under this transformation) the frozen scattering matrices of the two scatterers are equal at all times, and charge transport is the same in the two situations. On the other end the difference $\langle Q\rangle_1 - \langle Q\rangle_2$ is odd under reflection (as channel 1 is exchanged with channel 2), implying $\langle Q\rangle_1 - \langle Q\rangle_2 = 0$.

2.2. Adiabatic charge transport. A pumping process is considered adiabatic if the typical dwell time of a particle near the scatterer, the time during which the particle sees the scatterer, is much smaller than the adiabatic time scale $\tau \ll \omega^{-1}$, the typical time of variations of the scatterer; this means that the particle sees a quasi-static scatterer [**20, 39**]. In this regime one therefore expects the dynamical scattering matrix S_d to be related with the frozen on-shell scattering matrices $S(E,t)$. As the frozen scattering matrix $S(E,s)$ is a function of both time and energy, an important conceptual problem in understanding its meaning is represented by the uncertainty principle: a particle with a well defined time of passage has no well defined energy and vice-versa. In fact the variables on which the scattering matrix really depends are E and ωt, and the uncertainty $\delta E \delta\omega t \approx \omega$ is arbitrarily small in the adiabatic limit. This gives adiabatic charge transport a semiclassical flavour.

An useful instrument to analyse the semiclassical limit is provided by coherent states, and in fact it is possible to analyse the relation between S_d, S_f and $S(E,t)$ using coherent states [**9**]. Another possibility is the use of Weyl calculus (see Appendix A), where the operators on Hilbert space are associated to (in our case matrix valued) symbols, i.e. functions on phase space, which are power series in ω. We will see that the matrix $S(E,t)$ is the zeroth order part, called principal symbol, of the symbol associated with S_d.

Our discussion of adiabatic charge transport will therefore start with the description of classical pumping, in particular of the phase space underlying it and of the role of the classical time delay and energy shift. The description of adiabatic classical pumping is completed in Appendix B. We will then identify the symbols corresponding to the operators relevant for adiabatic charge transport, in particular we will describe the symbol corresponding to the density matrix ρ_{out} of the outgoing states. The derivation of the formulae (3.1), (3.2) and (3.4) will then reduce to the calculation of integrals over phase space, thanks to the trace formula (A.9).

2.2.1. *Classical pumping.* We proceed now to the description of classical pumps. We will first describe the phase space for the scattering states, then introduce the energy shift and the time delay and finally state the formula for the charge transport. The proof of this formula can be found in Appendix B. The relation between the energy shift and the expected charge transport is formally similar to the BPT formula. There is a big difference to the quantum case in that the energy shift cannot be determined by

static scattering data alone, which therefore do not characterize charge pumping even in leading order.

We picture each channel as an half-line $x > 0$. The phase space associated to a given channel is the half plane $\{(x,p)|x \geq 0\,,\ p \in \mathbb{R}\}$. We can describe it in terms of other coordinates (E,s), $E \geq 0$ such that E is the energy of the particle and t its time of passage at the origin. At time 0 particles with $t > 0$ are incoming and particles with $t < 0$ are outgoing. Assuming a dispersion relation $\epsilon(p) = \epsilon(-p)$, the velocity of the particle is $v = \epsilon'(p)$, and the change of coordinates is

$$E = \epsilon(p)\,, \qquad\qquad t = -\frac{x}{v}\,.$$

It is a canonical transformation, as $dx \wedge dp = dE \wedge dt$; the mapping is singular when $v = 0$.

The phase space Γ for n disconnected channels consists of n copies of the energy-time half plane

$$\Gamma = \bigcup_i^n \Gamma_i = \{(E,t,i)|E \geq 0\,,\ t \in R\,,\ i \in \{1,\dots,n\}\}\,.$$

The Hamiltonian is $h(E,t) = E$, and the flow $\Phi_s : \Gamma \to \Gamma$ generated by it acts as $\Phi_s(E,t) = (E, t-s)$, solving the canonical equation of motion

$$\frac{d}{dt}\Phi_s(E,t) = I(dh)|_{\Psi_s(E,t)}\,,$$

where $I : T^*\Gamma \to T\Gamma$ is the symplectic two-form. When we connect the channels through the pump, Γ still serves as phase space of the scattering states, and h still defines the energy in the channels: we denote by (E,t,i) the particle whose past asymptote is the free trajectory with this initial data; in an analogous way we can describe a particle by his future free trajectory (E',t',j). This way we avoid introducing the full phase space of the channels and the pump. Some particle may admit only one of the labels, as particle which are free in the past may get trapped in the pump, or particle which are free in the future may have been released from the pump. With this exception we have defined a bijection, the scattering map

$$S_d : \Gamma^- \to \Gamma^+ \qquad\qquad (E,t,i) \mapsto (E',t',j)\,,$$

where $\Gamma \backslash \Gamma^-$ contains the trajectories which are free in the past and get trapped, and analogously $\Gamma \backslash \Gamma^+$. For fixed i the function $j(E,t)$ is piecewise constant, and the map to (E',t') is symplectic (with the obvious exception of the regions concerned by the discontinuities). The inverse map S_d^{-1} provides the definition of the energy shift and of the time delay:

$$S_d^{-1} : (E',t',j) \mapsto (E,t,i) =: (E' - \mathcal{E}_d(E',t',j), t' - \mathcal{T}(E',t',j), i)\,. \tag{3.22}$$

Static scattering is energy conserving, implying $\mathcal{E}_d = 0$, and in static scattering the time delay does not depend on time of passage. For adiabatic scattering the energy shift is of order ω^1, we call $\mathcal{E}$ his leading order term, and the time delay is $\mathcal{T}_d = \mathcal{T} + O(\omega)$, where $\mathcal{T}$ is the time delay belonging to the frozen scatterer in effect at time equal to the time of passage t', on which it depends parametrically.

The fact that the map preserves volumes (following from Liouville theorem), together with the fact that derivatives with respect to time bring in a factor of ω now implies

$$\mathcal{E}' + \dot{\mathcal{T}} = O(\omega^2)\,. \tag{3.23}$$

The relation (3.23) shows that the $O(\omega)$ part of the energy shift is determined by static scattering data only up to an additive function of t' and j. This is in sharp contrast to the quantum mechanical case, where static scattering data (the frozen scattering matrix) totally determine the frozen energy shift.

The current is then written in terms of the energy shift as

$$\dot{Q}_j = \frac{1}{2\pi}\int dE g(E)\mathcal{E}(E,t,j)\,, \tag{3.24}$$

where $g(E)$ is the phase space density of space. In a semiclassical context $g(E)$ is associated with $\rho/2\pi$. The proof of (3.24) can be found in Appendix B. This proof will manifest the physical content of (3.24) and allow a semiclassical derivation of (3.1), where the relation of the current to the energy shift-time delay uncertainty is displayed.

2.2.2. *Adiabatic scattering.* The strategy for the proof of the formulae (3.1), (3.2) and (3.4) goes as follows: we first find the leading order symbols associated to the operators and then compute expectation values using the trace equality (A.9). The first main step is therefore the identification of the principal symbol of the dynamical scattering matrix, which we will see is the frozen on-shell scattering matrix. This identification will in turn allow for the one of the symbols associated to the energy shift and the density matrix of the outgoing states.

The result is

$$\sigma(S(t_0)) = S(E, t_0 + t) + O(\omega) \tag{3.25}$$

$$\sigma(\mathcal{E}_d) = \mathcal{E}(E,t) + O(\omega^2) \tag{3.26}$$

$$\sigma(\rho_{\text{out}}) = \rho(E) - \rho'(E)(\mathcal{E}(E,t) + O(\omega^2)) + \frac{1}{2}\rho''(E)\mathcal{E}^2(E,t) + O(\omega^3) \tag{3.27}$$

Since at $T = 0$ we have $\rho'(E) = -\delta(E - \mu)$, smallness in (3.27) is in the sense of distributions.

The argument for (3.25) goes through the frozen scattering operator, which is a zeroth order approximation of the dynamical scattering matrix, and whose exact symbol is

$S(E,t)$. In fact it holds true that

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

The matrix elements on both sides are significant if the difference $t-t'$ is small, within the order of the dwell time near the scatterer.

Next we use

$$|t,j\rangle = \frac{1}{\sqrt{2\pi}}\int dE \mathrm{e}^{\mathrm{i}Et}|E,j\rangle\,,$$

together with the definition (3.15) of the frozen on-shell scattering matrix (we recall that this very definition implies that the frozen S matrix conserves energy), to verify

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

which manifests indeed $S(E,t)$ as the principal symbol of the scattering matrix (see (A.3)), thus establishing (3.25) for $t_0=0$. The quantization of $S(E,t)$ then satisfies (3.14) as it must.

We then observe

$$\begin{aligned}\sigma^{(P)}(\dot S_d) &= 0\\ \sigma^{(SP)}(\dot S_d) &= \sigma^{(SP)}(-\mathrm{i}[H_0,S_d]) = -\mathrm{i}\{E,S(E,t)\} = \mathrm{i}\dot S(E,t)\,,\end{aligned}$$

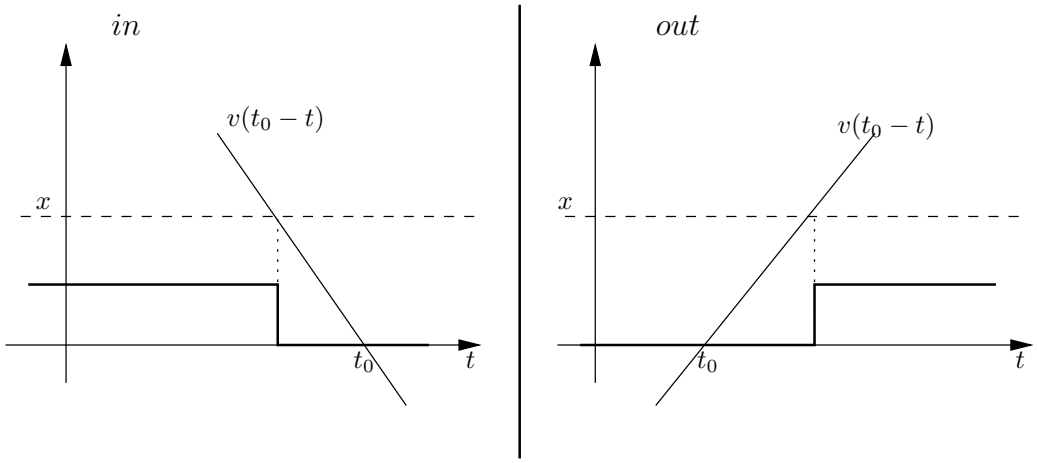
where $\sigma^{(P)}$, resp. $\sigma^{(SP)}$, denote the principal, resp. the subprincipal symbol. The second equation follows from (3.16) and the third from rule (A.6). This proves (3.26). (3.27) then follows by the the operator identity for the outgoing density (3.18) with the application of rule (A.7).

2.2.3. *Charge transport.* The (formal) derivation of the BPT formula is now in order: let $Q_j^{\mathrm{in/out}}(t_0)$ be the operator corresponding to counting the number of incoming resp. outgoing electrons in channel j that lie to the right of a point x at the point in time t_0. We choose x far away from the scatterer, but not too far away: x has to be such that the time the particle needs to travel the distance from the scatterer is long with respect to the dwell time and short with respect to the adiabatic time scale $\tau \ll |x/v| \ll \omega^{-1}$. The scattered particle will then be detected when the interaction with the pump has already finished and its motion is already essentially free, but at a time which is roughly the time of scattering (as measured by the pump cycle).

The symbol of $Q_j^{\mathrm{in/out}}(t_0)$ is a matrix valued step function (see Figure):

$$\sigma(Q_j^{\mathrm{in/out}}(t_0)) = P_j\theta(v(t-t_0)-x)\theta(\pm(t-t_0))\,,$$

where θ is the Heaviside step function and P_j is the matrix projection on channel j. In fact the the position of a particle with coordinates (E,t) at time 0 will be $-v(t-t_0)$ at



time t_0. Incoming particles at time t_0 have $t > t_0$. The associated incoming/outgoing current operators are the rate of change of the operators $Q_j^{\text{in/out}}(t_0)$:

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

and the symbols associated to them are:

$$\begin{aligned}\sigma(\dot{Q}_j^{\text{in/out}}(t_0)) &= P_j\{h(E,t), \theta(v(t-t_0)-x)\theta(\pm(t-t_0))\} + O(\omega^2)\\ &= P_j\delta(t_0 - t - \frac{x}{v})\theta(\pm(t-t_0)) + O(\omega^2)\,,\end{aligned} \tag{3.28}$$

as $t = t_0$ falls outside the support of the first Heaviside function. x is the position where the ammeter is placed, and leads to a modification of the time t_0 where the particle is detected. The assumptions on x have precisely the role to ensure that this modification is not relevant on the macroscopic time scale defined by the cycle of the pump. We therefore drop x from now on. The expectation value of the current is

$$\langle \dot{Q}_j \rangle(t_0) = \mathrm{Tr}(\rho_{\text{out}}\dot{Q}_j^{\text{out}}(t_0)) + \mathrm{Tr}(\rho\dot{Q}_j^{\text{in}}(t_0)) = \mathrm{Tr}(\delta\rho\dot{Q}_j^{\text{out}}(t_0))\,,$$

where $\delta\rho = \rho_{\text{out}} - \rho$. The trace is evaluated as an integral over phase space using (A.9) (the symbols are given by (3.27), (3.28)), which leads to the BPT formula

$$\begin{aligned}\langle \dot{Q}_j \rangle(t_0) &= -\frac{1}{2\pi}\int dE dt \rho'(E)\mathcal{E}_{jj}(E,t)\delta(t-t_0) + O(\omega)\\ &= -\frac{1}{2\pi}\int dt \rho'(E)\mathcal{E}_{jj}(E,t_0)\,.\end{aligned}$$

2.2.4. *Dissipation.* To derive the equation (3.2) for the dissipation we proceed in the same way as in the previous paragraph: we introduce $D_j^{\text{in/out}}$, the operator associated to the incoming/outgoing excess energy deep into channel j, we find the symbol corresponding to it and evaluate the trace producing the expectation value as an integral

over phase space. The excess energy is the energy measured with respect to the Fermi energy

$$D_j^{\text{in/out}} = \frac{1}{2}[Q_j^{\text{in/out}}, H_0 - \mu]_+ ,$$

where $[\cdot,\cdot]_+$ denotes the anticommutator. The symbol corresponding to the excess energy is

$$\sigma(D_j^{\text{in/out}}) = P_j(E-\mu)\theta(v(t-t_0)-x)\theta(\pm(t-t_0)) + O(\omega^2) .$$

The dissipation current in channel j is the time derivative of the excess energy

$$\dot{D}_j^{\text{in/out}} = \mathrm{i}[H, D_j^{\text{in/out}}] = \dot{E}_j^{\text{in/out}} - \mu \dot{Q_j^{\text{in/out}}} ,$$

(where $\dot{E}_j = (1/2)[H_0,[H_0,Q_j]_+]$) and the symbol associated to it is therefore

$$\sigma(\dot{D}_j^{\text{in/out}}) = P_j(E-\mu)\delta(t_0 - t - \frac{x}{v})\theta(\pm(t-t_0)) + O(\omega^2) .$$

The expectation value of the dissipation current is then found to be, in analogy to the calculation in the previous paragraph

$$\langle \dot{D}_j^{\text{in/out}} \rangle = \mathrm{Tr}(\delta\rho \dot{D}_j^{\text{out}}) . \tag{3.29}$$

We calculate (3.29), again with (A.9), for temperatures $T \lesssim \sqrt{\omega/\tau}$. At low temperatures ρ' is concentrated near μ, we approximate therefore the energy shift linearly around μ. For the therm proportional to ρ' in (3.27) we find

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

and for the term proportional to δ'' we find

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

This result is remarkable as we obtain a result which is valid to order ω^2 by making two assumptions valid only to order ω: we approximate $\mathcal{E}_d$ by $\mathcal{E}$ (see (3.26)) and then we approximate $\mathcal{E}$ by its linear value around μ. Had we applied this approximations to the single terms $\langle \dot{E}_j \rangle$ and $\mu\langle \dot{Q}_j \rangle$ we would have determined them to order ω only. This is ascribed to the fact that the dissipation current obeys the lower bound (3.3), which is saturated by an outgoing density with full occupation density for $E < \mu$ and empty thereafter [**8**], for which the dissipation, as given by the right hand side of (3.3), is order ω^2. The actual outgoing occupation density at $T = 0$ is an ω approximation of this minimiser. The deviation from the minimal value is quadratic in the distance from the minimizer, and therefore of order ω. This argument has to be made a bit more precise, as deviation from the minimal value are not necessarily quadratic in perturbations around the minimizer. The first necessary condition for this to hold is that the minimal value is attained in the interior of the region R defined by the constraints, in our case $0 \le \rho \le 1$.

This is not the case for us, as the minimizer lies on the boundary of R; this is however not a problem, as the perturbation we are considering,

$$\rho(E) \to \rho(E - \mathcal{E}) \,, \tag{3.30}$$

does not point away from the boundary (neither (3.30) nor the perturbation in the opposite direction, obtained substituting $\mathcal{E}$ by $-\mathcal{E}$, violate the constraint $0 \leq \rho \leq 1$). The second necessary condition is the Hessian of the functional to minimize to be a bounded operator. This is again not the case, as the Hessian has arbitrarily high modes corresponding to changing the occupation density of particles with arbitrarily high energy. This is again not a problem, as the perturbation (3.30) modifies the occupation density only around the Fermi energy.

2.2.5. *Entropy and noise currents.* The density and noise currents introduce a new element: their dependence on the density matrix is given through a non-linear function h. In both cases the function $h(x) = 0$ for $x = 0, 1$. We will use this fact to show that for $\omega \ll T \ll \sqrt{\omega/\tau}$ the currents are given by

$$\dot{s}_j(t, \mu, T) = \frac{\beta}{2\pi} \Delta\mathcal{E}_j^2(\mu, t) \int_0^1 dx h(x) \,, \tag{3.31}$$

where $\Delta\mathcal{E}_j^2(\mu, t)$ has been defined in (3.8). The integral gives $1/2$ for the entropy current and $1/6$ for the noise current.

We complete the discussion of entropy and noise currents with the derivation of (3.31). The condition $\omega \ll T$ makes it possible to consider electrons with a fixed time of passage, provided the time resolution is short compared to ω^{-1} but long compared to T^{-1}. The state $\rho_{\mathrm{out},j} = P_j \rho_{\mathrm{out}} P_j$ is then given (see (3.27)) by

$$\begin{aligned} \rho_{\mathrm{out},j}(E) &= P_j \rho(E) P_j - \rho'(E) P_j \mathcal{E}(E,t) P_j + \frac{1}{2}\rho''(E)(P_j \mathcal{E}(E,t) P_j)^2 + \frac{1}{2}\rho''(E)\Delta\mathcal{E}_j^2(E,t) \\ &= \rho_j(E - \mathcal{E}(E,s)) + \frac{1}{2}\rho''(E)\Delta\mathcal{E}_j^2(E,t) \,. \end{aligned}$$

The entropy/noise current (3.4) is

$$\frac{1}{2\pi}\int dE((h\circ\rho)(E - \mathcal{E}_{jj}(E,t)) - (h\circ\rho)(E) + \frac{1}{4\pi}\int dE (h'\circ\rho)(E)\rho''(E)\Delta\mathcal{E}_j^2(E,t) \,. \tag{3.32}$$

In these integrals $\mathcal{E}_{jj}$ may be considered constant in E (with the value evaluated at $E = \mu$) because of the condition $T \ll \sqrt{\omega/\tau}$.

As a consequence, the first integral is zero and we may pull $\Delta\mathcal{E}_j^2(\mu, t)$ out of the second. The calculation reduces to that of the integral

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

where the substitution is made possible by a property of the Fermi function, $\rho' = -\beta\rho(1 - \rho)$, implying $\rho''/\rho' = -\beta(1 - 2\rho)$. Equation (3.31) follows by partial integration (as $h(0) = h(1) = 0$). This completes the derivation of entropy and noise currents

at positive temperature. Why does this procedure not work for small temperatures? The mathematical reason is that the functions ρ' and ρ'' become distributions and it is not possible to multiply them. As a consequence expressions like (3.32), which are nonlinear in ρ, do not make any sense. For the derivation to work we need ρ to be smooth on the energy scale defined by the adiabatic frequency ω.

This is a reflection of the fact that at $T = 0$ time correlations decay slowly, and the entropy/noise currents, having a nonlinear dependence on ρ, display memory effects on the time scale T^{-1}.

2.3. The BPT formula as a theorem. We now present a mathematical setting in which it is possible to state the BPT formula (3.1) as a theorem [**11**]. The Hilbert space

$$\mathcal{H} = \mathcal{H}_0 \oplus L^2(\mathbb{R}_+, \mathbb{C}^n)$$

consists of a pump proper connected to n channels, described as half-lines. The Hilbert space of the pump is not further specified, although the assumption (3.34) confers to the pump the role of an abstract finite box [**59**]. The operators Π_j, $j = 0, 1, \ldots, n$ denote the projection onto the pump Hilbert space for $j = 0$ and onto the j-th channel (the j-th copy of L^2 in $\oplus_1^n L^2(\mathbb{R}_+) = L^2(\mathbb{R}_+, \mathbb{C}^n)$).

The evolution is the non autonomous one generated by the family of Hamiltonians $H(s) = H(\omega t)$, where s defines the time as measured by the pump cycle. Eventually the adiabatic limit $\omega \to 0$ is taken. The assumptions on $H(s)$ are the following:

$$H(s) - H(s') \qquad \text{is bounded and smooth in } s, \tag{3.33}$$

$$\|(H(s) + i)^{-m}\Pi_0\|_1 \leq C \qquad \text{for all } s \text{ and some } m \in \mathbb{N}, \tag{3.34}$$

$$H(s)\psi = -\frac{d^2\psi}{dx^2} \qquad \text{for } \psi \in C_0^\infty(\mathbb{R}_+, \mathbb{C}^n), \tag{3.35}$$

$$\sigma_{pp}(H(s)) \cap]0, \infty[= \emptyset \tag{3.36}$$

$$H(s) = H_- \qquad \text{for } s \leq 0, \tag{3.37}$$

where $\|\cdot\|_1$ denotes the trace class norm over $\mathcal{H}$. The assumptions have a clear physical meaning: assumption(3.35) states that the particle move freely in the channels, and, together with condition (3.33) that the changes in $H(s)$ are confined to the pump proper

$$H(s') - H(s) = (H(s') - H(s))\Pi_0\,;$$

assumption (3.36) states that there are no eigenvalues embedded in the continuous spectrum, and (3.37) states that the pump is time-independent for $t < 0$, and allows one to impose that the electrons are in equilibrium as long as the pump is at rest. This is achieved by choosing as initial state at some $t < 0$ a density matrix of the form $\rho(H_-)$, where ρ is a regular function with $\text{supp}(d\rho) \subset]0, \infty[$. An example is the Fermi sea, with $\rho(\lambda) = \theta(\mu - \lambda)$.

In order to define the current, the authors consider the operator

$$A = 0 \oplus \frac{1}{2i}\big(\frac{d}{dx}v(x) + v(x)\frac{d}{dx}\big)$$

where $v : [0, \infty[\to \mathbb{R}$ is a monotonous function, which is equal to zero near the pump and to x deep inside the channels. As $A = A^*$ commutes with P_j, it makes sense to define the operators $A_j = A\Pi_j$. In practice this operator weighs the momentum of the particle, which can have either sign, by its distance $x > 0$ from the pump. It can therefore distinguish between incoming and outgoing states, corresponding to spectral subspaces $A < -a$ and $A > a$ respectively, for some fixed, large $a > 0$.

The detection of a particle may be realized deep inside lead j by the operator

$$Q_j(a) = f(A_j - a) + f(-A_j - a)\,,$$

where f is a smooth switch function: $f(\lambda) = 0$ for $\lambda < -1$, $f(\lambda) = 1$ for $\lambda > 1$. The current operator is then defined as

$$I_j(a) = \mathrm{i}[H(s), f(A_j - a) + f(-A_j - a)] =: I_{j+}(a) + I_{j-}(a)\,. \tag{3.38}$$

The number a determines the position where the ammeter is placed (the definition of A implies that the ammeter is placed a fixed number of wavelength away from the pump, rather that a fixed position; the bigger the wavelength, the more distant the ammeter. If one considers a small energy interval, let us say near the Fermi energy, then also the position of the ammeter is essentially fixed). The BPT formula would describe the current as

$$\lim_{a\to\infty}\lim_{\omega\to 0}\omega^{-1}\langle I\rangle_j(s, a, \omega) = -\frac{\mathrm{i}}{2\pi}\int_0^\infty d\rho(E)\big(\frac{dS(E,s)}{ds}S(E,s)^*\big)_{jj}\,. \tag{3.39}$$

In fact the theorem is stated in a slightly modified form with respect to (3.39) as the current needs IR and UV cut-offs. The reason for this is that in both the IR and UV regimes the dwell time near the pump may become arbitrarily large, whence the impossibility of an adiabatic theorem to hold. If the definition (3.38) is changed accordingly, introducing the necessary cut-offs, then (3.39) is a theorem, and can be proven in full mathematical rigour.

We will not give the details of the proof, instead we comment on the similarities between this rigorous description and the formal derivation we have given above. The order of the limits in the statement (3.39) means that the physical picture we had in mind above is the correct one: the ammeter is placed such that the particle are seen well after the interaction with the pump has terminated, as a is large. It is however not too far: the particles have to be detected essentially at the time of scattering s (or equivalently ωt) as measured by the pump cycle. This separation of time scales is realized by the fact that the adiabatic limit is taken before the limit $a \to \infty$. As in the derivation of paragraph 2.2 the current operator is split into two parts, an incoming and an outgoing one, which are distinguished by the fact that the outgoing one measures particle that

have already been scattered.

One central element of the proof is the existence of propagation estimates, ensuring that the picture about the separation of time scales given above does in fact happen: the particles reach the ammeter a finite time after the scattering. Propagation estimates guarantee moreover that the particles do not get stuck in the pump, ensuring that way that they see a frozen scatterer in the adiabatic limit; furthermore they cause the rigidity of the result (3.39) with respect to all arbitrary choices, such as the choice of the functions v, or f or of the past time-independent Hamiltonian H_-, that disappear in the limit.

In the adiabatic limit is then possible to relate the current, a first order quantity, to frozen data. This is remarkable, because it is an example of an adiabatic theorem for open gapless systems, and unlike other results of this kind do not treat the evolution of the subspace corresponding to an embedded eigenvalue.

The expectation value of the current is then related to frozen quantities, which reduce to the frozen scattering data in the limit $a \to \infty$.

3. The geometry of charge transport

In this section we explain the geometric content of charge transport [**10**] in the formalism of the scattering approach. The rows of the matrix $S(E,t)$ are unit vectors in $\mathbb{C}^n$ and the charge transport can be understood in term of geometric properties of these vectors. We denote by

$$|\psi_j\rangle = (S_{j1}, S_{j2}, \ldots, S_{jn})^T$$

the transpose of the j-th row of the frozen on-shell scattering matrix. The BPT formula for the charge transported in channel j takes the form

$$2\pi\langle Q_j\rangle = \mathrm{i}\langle\psi_j|d\psi_j\rangle\,. \tag{3.40}$$

We first observe that (adiabatic) transport is geometric: the charge transported in a process depends only on the path this process describes in the space of scattering matrices, and not on the rate with which the path is traversed. The formula (3.40) states that the charge transport equals the change in phase of the vector $|\psi_j\rangle$, as measured by the one-form on the right-hand side, the global angular form, which is formally the same as Berry's connection [**14**]. We will comment on the different role it plays here with respect to adiabatic theory. Remarkably, when the path in scattering matrices is closed, as in the case of a complete pump cycle, charge transport is computable without knowledge of the global phase, by means of the curvature of the global angular form. In contrast to other cases, this integral needs not to be quantized. We will however single out a class of pump operations producing quantized transport. This class of pump operation will be characterized geometrically on one side, on the other side we will see that this characterization is equivalent to the notion of optimality. The quantization of

transport will therefore be related to the minimization of the dissipation.

3.1. The global angular form. In analogy to Riemannian geometry, where the connection (or equivalently the parallel transport) allows to compare the orientation of vectors in different tangent spaces, the global angular form allows to intrinsically define the change in phase of a vector $|\psi_j\rangle$ on a path in parameter space. The information contained in an unit vector in $\mathbb{C}^n$ may be decomposed in two parts: the subspace in $\mathbb{C}^n$ to which it belongs, and a phase γ. It is however impossible to recover the vector from this information (or analogously it is impossible to define the phase), without the (arbitrary) definition of a reference vector in the subspace.

In spite of this it is possible to define the change in phase on a path intrinsically, i.e. without referring to a choice of reference vectors on the path. This is done by means of the parallel transport. For this to be true, the change in phase defined by parallel transport should be the right one for "vertical" paths happening constantly in a given subspace $|\psi_j\rangle = \mathrm{e}^{\mathrm{i}\theta}|\psi_0\rangle$, where the change in phase is clearly $\int d\theta = -\mathrm{i}\int\langle\psi_j|d\psi_j\rangle$. A natural choice is then to say that a vector is parallel transported if there is no motion in the direction $|\psi_j\rangle\langle\psi_j|$.

The equation of parallel transport is

$$|\psi_j\rangle\langle\psi_j|d\psi_j\rangle = 0, \tag{3.41}$$

where the left hand side is the covariant derivative. Now, for a general motion, the global angular form

$$-\mathrm{i}\langle\psi_j|d\psi_j\rangle \tag{3.42}$$

measures the deviation from parallel transport. We can now compute the deviation from parallel transport for any path, open or closed. The geometric content of BPT formula is that the charge transport is $-1/2\pi$ times the accumulated phase along the path.

We phrase the above considerations in more geometric language: the pump typically operates by periodically changing some parameters $(\varphi_1, \ldots, \varphi_n)$, we denote parameter space by M. The j-th row of the scattering matrix defines then a map $\tilde{f}$ from parameter space M to $S^{2n-1} \ni |\psi_j\rangle$, and indirectly a map f to $\mathbb{C}P^n \ni |\psi_j\rangle\langle\psi_j|$. The sphere S^{2n-1} is given a $U(1)$ bundle structure on $\mathbb{C}P^n$ by the Hopf fibration $|\psi_j\rangle \mapsto |\psi_j\rangle\langle\psi_j|$, and the pull-back f^* of this bundle is a trivial $U(1)$ bundle on M. Although the bundle is topologically trivial, as $\tilde{f}$ provides with a global section, it possesses an interesting geometry, describing charge transport through the global angular form.

The expression for the global angular form (3.42) is familiar from the context of adiabatic connections and Berry's phase [**14**]. There is however a difference between Berry's phase associated to a quantum state $|\psi\rangle$ and the phases that arise in the study of the S matrix. In the usual Berry's phase setting one starts with a circle of Hamiltonians

to which one associates a family of projections, say to the ground state, $|\psi\rangle\langle\psi|$. To represent these by means of a circle of eigenvectors $|\psi\rangle$ one needs to arbitrarily choose a reference phase for every point on the cycle. Physical evolution picks up his own phase. In the adiabatic limit ([**30**]) this phase is known to be given by the parallel transport $\langle\psi|d\psi\rangle = 0$ (one can get rid of the dynamical phase by setting the ground state energy to 0), and Berry connection measures the difference between the phase chosen by physical evolution and the reference phase. For a complete closed cycle the reference phase returns to its original value, and Berry's connection measures the change in phase of the physical wave function.

A cycle of the pump, in contrast, determines a circle of vectors $|\psi_j\rangle$. No choice of reference phases has to be made, as the phases are all given by the scattering matrix. The vector $|\psi_j\rangle$ returns to his original value at the end of the cycle. The BPT formula then states that the charge transport is obtained comparing this given phase with the one determined by parallel transport, and Berry's connection still measures this difference. Only the interpretations are not the same: instead of measuring the amount to which physical parallel evolution fails to close on itself, now it measures the amount to which physical closed evolution fails to be parallel.

3.2. The curvature two-form. Brouwer [**16**] observed the following remarkable fact: the charge transport for a complete cycle of the pump (or equivalently the dc component of transport) can be calculated without knowledge of the global phase of $|\psi_j\rangle$, relying only on $|\psi_j\rangle\langle\psi_j|$. This is done applying Stokes theorem to the integrated charge transport described by the BPT formula: for a closed path in parameter space ∂D, $D \subset M$, one finds

$$2\pi\langle Q_j\rangle = \mathrm{i}\int_{\partial D}\langle\psi_j|d\psi_j\rangle = \mathrm{i}\int\langle d\psi_j|d\psi_j\rangle\,, \tag{3.43}$$

(we emphasize that this quantity is not an integer as a rule). The integrand on the right hand side

$$\langle d\psi_j|d\psi_j\rangle = \sum_{k<l}(\langle\partial_{\varphi_k}\psi_j|\partial_{\varphi_l}\psi_j\rangle - \langle\partial_{\varphi_l}\psi_j|\partial_{\varphi_k}\psi_j\rangle)d\varphi_k\wedge d\varphi_l$$

may be rewritten as

$$\mathrm{i}\langle d\psi_j|d\psi_j\rangle = -\mathrm{i}(dS\wedge dS^*)_{jj} = -\mathrm{i}\,\mathrm{tr}(\hat{P}_j d\hat{P}_j\wedge d\hat{P}_j\hat{P}_j) \tag{3.44}$$

where $\hat{P}_j$ is the projection to the states feeding channel j

$$\hat{P}_j = S^*P_jS = |\psi_j\rangle\langle\psi_j|\,.$$

The right-hand side of (3.44) is the trace of the curvature associated to the covariant derivative $\hat{P}_j d$ (see [**4**], Section 9.5).

Brouwer's formula applies Stokes theorem to a closed path in parameter space. For a closed cycle of the pump, time lives on the unit circle $t \in S^1$, and the charge transport is

obtained integrating the energy shift over S^1 at the Fermi energy. This is one of the two disconnected parts of the boundary of the cylinder $C = [0, \mu] \times S^1$ in energy-time space. Applying Stokes theorem to this domain one obtains a description of charge transport highlighting the role played by the time delay-energy shift uncertainty $\Omega = \mathrm{i}[\mathcal{T}, \mathcal{E}]$. This formula also clarifies that although the transport is calculated through quantities evaluated at the Fermi energy alone, it is attributed to all the states in the Fermi sea. The formula is obtained, assuming that there are no semi-bound states, $\mathcal{E}(0,t) = 0$ (see Appendix B), by application of Stokes theorem

$$2\pi\langle Q_j\rangle = \int_{S^1} dt(\dot{S}S^*)_{jj}(\mu,t) = \int_{\partial C}(dSS^*)_{jj}(E,t) = \int_C \Omega_{jj}(E,t)\,, \tag{3.45}$$

where

$$\Omega_{jj}dE\wedge dt = d\mathcal{E}_{jj}\wedge dt + dE\wedge d\mathcal{T}_{jj} = -\mathrm{i}(dS\wedge dS^*)_{jj}\,,$$

so that the time delay-energy shift uncertainty has the geometric interpretation of curvature in energy-time space.

The difference between (3.45) and Brouwer's formula is the domain of integration: a disc in parameter space for (3.43) and a cylinder in energy time space here. However, since $\mathcal{E}(0,t) = 0$, the lower circle may be pinched to a point, and the cylinder becomes a disc. $-\mathrm{i}(dS\wedge dS^*)_{jj}$ is the trace of the curvature of the connection $\hat{P}_j d$, or of its connection one-form $\mathcal{E}_{jj}dt - \mathcal{T}_{jj}dE$. Similar equations are found in the context of the Quantum Hall effect (see e.g. [**4**] Chapter 10), the basis manifold being a torus of fluxes, but unlike there the integral does not define a Chern number, as the integration manifold has a boundary (obviously one cannot identify the two boundaries of the cylinder).

3.3. The two channel case. The description of the two channel case is further simplified by the fact that the projective space $\mathbb{C}P^n$ is identified with S^2 by stereographic projection. The first row of the scattering matrix $|\psi_1\rangle = \begin{pmatrix} r \\ t' \end{pmatrix}$ lives in S^3. The projection associated to $|\psi_1\rangle$ may be identified with a point on the sphere S^2 by

$$|\psi\rangle\langle\psi| = \frac{1+\hat{n}\cdot\vec{\sigma}}{2}\,, \tag{3.46}$$

where $\hat{n}$ is a unit vector and $\vec{\sigma}$ denotes the triplet of Pauli matrices. The trace of the curvature

$$\omega(\hat{n}) := -\mathrm{i}\,\mathrm{tr}(\hat{P}_j d\hat{P}_j\wedge d\hat{P}_j\hat{P}_j)$$

is then a two-form on S^2, invariant under rotations

$$\tilde{n}(|\psi\rangle\langle\psi|) = R\hat{n}(|\psi\rangle\langle\psi|)\,,$$

where $R\in SO(3)$ (by $\tilde{n}(|\psi\rangle\langle\psi|) = \hat{n}(U|\psi\rangle\langle\psi|U^*)$, $U\in SU(2)$), and is therefore a multiple of the area form. Considering the process $|\psi\rangle = \mathrm{e}^{\mathrm{i}\lambda}|\psi_0\rangle$ with λ going from 0 to

2π we find

$$2\pi\langle Q_1\rangle = 2\pi = \int_{S^2} \omega\,,$$

i.e. ω is $1/2$ of the area form (this is known from the study of spins in an adiabatic changing magnetic field, see [**4**] section 10.2, where the $1/2$ reflects the fact that spin interfere destructively after a complete 2π rotation in physical space).

The unit vector $\hat{n}$ as defined by (3.46) is related to $z = r/t' \in \mathbb{C}P^1 = \mathbb{C} \cup \{\infty\}$ by stereographic projection

$$\hat{n} = (2\mathrm{Re}(r\bar{t}'), 2\mathrm{Im}(r\bar{t}'), |r|^2 - |t'|^2) = (\frac{2\mathrm{Re}(z)}{|z|^2+1}, \frac{2\mathrm{Im}(z)}{|z|^2+1}, \frac{|z|^2-1}{|z|^2+1})\,.$$

The fact that the charge transport in a cycle may be computed without knowledge of the global phase amounts to the fact that the curvature $\mathrm{i}(d\bar{r}dr + d\bar{t}'dt')$ is entirely expressed in term of z:

$$\mathrm{i}(d\bar{r}dr + d\bar{t}'dt') = \mathrm{i}\frac{d\bar{z}dz}{(1+|z|^2)^2}\,.$$

There is however an ambiguity, related to the fact that the mapping from parameter space to the sphere S^2 is in general not bijective. In fact only the fractional part of the charge transport is obtained integrating on the sphere. How can one then recover the full description of charge transport without referring to the global phase? The integral part of the charge transport is given by the degree of the mapping from parameter space to the sphere, i.e. it is calculated counting how many times a value z (for instance $z = 0$) is taken by the map $f : M \to \mathbb{C}P^1$ (counting with sign and multiplicity). The fact that the fractional part of charge transport is calculated with an area integral on the sphere means that if the whole cycle happens with a fixed value of r/t' (for instance by having $|r| = 1$ for the entire cycle), the fractional part is zero and charge transport is quantized. The quantized value of transport is then for instance obtained by counting how many points are there in parameter space, where the scattering matrix is reflectionless at the Fermi energy. This is further discussed and exemplified in Section 4.

3.4. The issue of quantization. As already stated, the topology of the above description is trivial. This fact rules out the hypothesis that charge transport in open quantum pumps, described by the BPT formula, is quantized by its relation to a Chern number. This does not rule out the possibility that for some pumping cycles other mechanisms ensure the charge transport to be quantized. In this paragraph we want to clarify these two facts. In next paragraph we will then see how the issue of quantization is related to the notion of optimality.

We begin by reminding that the Hopf fibration

$$\begin{aligned} \pi : S^{2n-1} &\longrightarrow \mathbb{C}^n \\ |\psi\rangle &\longmapsto |\psi\rangle\langle\psi| \end{aligned}$$

gives the unit sphere $S^{2n-1} \subset \mathbb{C}^n$ the structure of a $U(1)$ principal bundle over complex projective space $\mathbb{C}P^n$.

Chern numbers typically arise in transport theory as follows: given a family of Hamiltonians $H(\Phi)$, depending on some parameters $\Phi \in M$, M a closed surface (say a sphere or a torus), an eigenvalue $e_j(\Phi)$ defines a map f from M to $\mathbb{C}P^n$. The pullback of the Hopf fibration under this map is a $U(1)$ principal bundle over M, with local geometry and possibly non-trivial topology. The integrated curvature is a Chern number, it is often identified with transport coefficients, and can be nonzero.

In quantum pumps the situation is different: the scattering matrix $S(\mu, t)$ defines a map $\tilde{f}$ directly to S^{2n-1}, giving therefore a trivialization of the bundle. As a consequence all Chern numbers have to vanish. Besides, charge transport is the integral of the Chern character $-\mathrm{i}\langle d\psi | d\psi\rangle$ over a surface with boundary, and cannot be a Chern number.

There can however be other reason for the charge transport to be quantized: if the pumping process is such that the projection $|\psi\rangle\langle\psi|$ is fixed, then

$$|\psi\rangle = \mathrm{e}^{\mathrm{i}\theta}|\psi_0\rangle\,, \tag{3.47}$$

and the charge transport is the winding number of $\mathrm{e}^{\mathrm{i}\gamma}$ (or, alternatively, the curvature can be computed in term of $\hat{P}_j = \pi(|\psi\rangle)$, and the integral (3.43) calculated on $\pi(D)$. The fact that the projection is fixed means then $\partial\pi(D) = \emptyset$, which again shows that the charge transport is an integer).

3.5. Quantization and optimality. In this paragraph we give the geometric description of the equations (3.2) and (3.4) describing dissipation and noise. While charge transport and minimal dissipation are functions of the motion in the fibers, the excess dissipation and noise are associated to motion in the base. Optimal pumps, saturating the bound (3.3) on the dissipation, happen therefore with a fixed projection $|\psi_j\rangle\langle\psi_j|$, and transport a quantized charge by the argument of the previous paragraph. Moreover these are the only pumps for which the variance of transport vanishes. We have therefore attained a complete understanding of the equivalence between optimality and quantization of transport.

This is seen as follows: the j-th row of the matrix of energy shift is the velocity of $|\psi_j\rangle$ in S^{2n-1}. As we have seen, the term $\mathcal{E}_{jj}$ is the component of the velocity in the fiber, as defined by parallel transport $\langle\psi_j|d\psi_j\rangle$. The terms $\mathcal{E}_{jk}$, $k \neq j$ give the projection of the velocity to the base $\mathbb{C}P^n$

$$\mathcal{E}_{jk} = \langle\psi_k|\dot{\psi}_j\rangle = \langle\psi_k|(1 - |\psi_j\rangle\langle\psi_j|)|\dot{\psi}_j\rangle \qquad \text{for } j \neq l\,.$$

The charge transport and the minimal dissipation $|\mathcal{E}_{jj}|^2/4\pi$ are both functions of the velocity in the fiber, while the excess dissipation

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

is the velocity squared associated with motion in the base. In particular, the bound (3.3) is saturated if and only if the pump cycle is of the form (3.47). Optimal quantum pumps transport therefore an integer number of charges per cycle. Equivalently, another necessary and sufficient condition for optimality is the vanishing of noise at $T > 0$ (3.4) or at $T = 0$ (3.54); this means that the charge transport is not just an integer in expectation value, but is actually quantized in every cycle.

4. Examples

In this section we give some examples. Quantum pumping, as described by the BPT formula, is clearly a wave phenomenon: transport is attributed to changes in the phases of the scattering matrices, and manipulations of transmission and reflection probabilities only, leaving phases unchanged, produces no transport. Transport is therefore attributed to interference effects. On the other hand the derivation given in Paragraph 2.1 of the BPT formula in the two channel case shows that classical reasoning, where the pump is viewed as a particle pump, is efficient and provides some insight in the pumping mechanism. In the first two examples discussed in this section this is again the case: the pumping processes may be analysed from the particle and from the wave point of view. The particle point of view is more intuitive, but it does not translate to a quantitative description without making reference to some wave aspect. Analysing the phases appearing in the BPT formula one gets then a complete description of the transport achieved by the pump. Combining the two different insights one then gets a clear understanding of the pumping mechanism.

We then proceed with two further discussions: the first is an exemplification of the geometric construction in the two channel case presented in Paragraph 3.3, where the bicycle pump (4.1) is further discussed; the second shows that in the classical case time-independent scattering data alone cannot determine the energy shift, with the example of classical scattering from a battery.

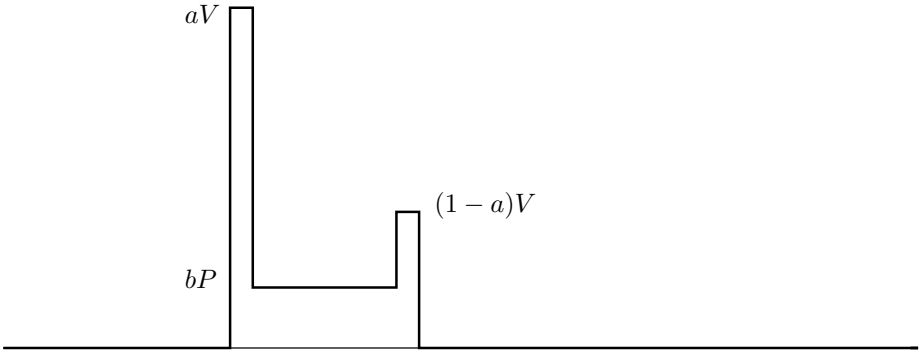
4.1. The bicycle pump. The first example we show is the quantum analogon of a bicycle pump. In an ordinary bicycle pump the opening and closing of the valves is synchronized with the action of the piston, so that what is aspired from one side is expelled at the other side. The particle interpretation of the pump corresponds to this picture, and is therefore simple and intuitive. The wave point of view is more subtle: we will see that transport is attributed to manipulations of the Galilean shift parameter

α and of the Birman-Krein term γ.

The synchronized action of valves and piston is realized by potentials of the form (see Figure)

$$V_{a,b}(x) = \begin{cases} 0 & x < 0 \\ Va & 0 \le x < \delta \\ bP & \delta \le x < L \\ V(1-a) & L \le x < L + \delta \\ 0 & l + \delta \le x \end{cases},$$

with (a, b) parcourring the boundary of the unit square $[0, 1] \times [0, 1]$. We choose the



length of the pump to be equal an integer number n of Fermi half-wavelengths $L = nk_F/\pi$, the height of the piston $P = 10\mu$, the valves thin, $\delta \ll \pi/k_F$, and impenetrable $V\delta \gg k_F/\pi$.

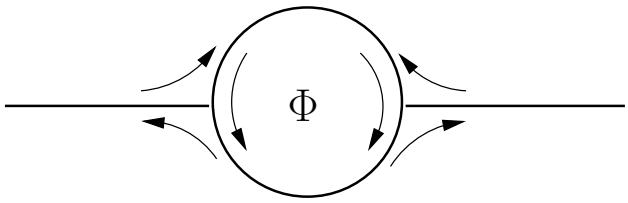
The particle interpretation really corresponds to a bicycle pump: as the piston comes down, particles enter the pump from the right, then the left valve closes, the right one opens an the particles are expelled to the right. As the length of the pump is chosen to accommodate n particles, the pump transports n particles per cycle.

We now pass to the BPT description of transport as realized by the bicycle pump: as at any moment at least one of the valves is closed, the scattering matrix is transmissionless for the whole cycle (at first sight the fact that transport is realized with a constantly transmissionless pump may seem odd; however this is exactly what happens in the classical case: a good pump has valves that do not leak). Although the pump works by manipulation gate voltages, the wave interpretation of the bicycle pump is through the Galilean shift parameter α and the Birman-Krein term γ.

We start the cycle at $(a, b) = (0, 1)$: there the piston imposes a Dirichlet condition at $x = 0$, whence $r = -1$, and the right valve imposes a Dirichlet condition at $x = L$, so $r' = -1$. As b goes from 1 to 0, the right valve stays closed and $r' = -1$ throughout. This implies $d\alpha = d\gamma$. Meanwhile the piston comes down, and the waves coming from the right enter more and more the pump. When $b = 0$ the left barrier has been effectively shifted a distance L to the right, so that r accumulates a total phase n. The

segment with $b = 0$, a going from 0 to 1, does not change the scattering matrix: as the pump length is equal to an integer number of Fermi half-wavelengths, a Dirichlet condition at $x = 0$ is equivalent to a Dirichlet condition at $x = L$. The first half of the cycle has produced a charge transport $\langle dQ\rangle_1 = -n$, $\langle dQ\rangle_2 = 0$. The remaining half of the pump cycle is examined in an analogous way, resulting in a transport $\langle dQ\rangle_1 = 0$, $\langle dQ\rangle_2 = n$. The charge transport is quantized, in agreement with the discussion of the previous section: the boundary of the unit square is mapped to a point (the north pole) on the unit sphere. The pump is therefore optimal. The quantized value n is the degree of the mapping from the interior of the unit square to S^2: there are n points (with $a = 1/2$, b such that $\frac{k_F}{\sqrt{\mu - bP}} = m < n$, $m \in \mathbb{N}$) where the frozen scattering matrix is reflectionless (analogously there are n such points on the energy time cylinder $[0, \mu]\times S^1$).

4.2. The U-turn pump. The U turn pump is an optimal pump which is an highly schematic representation of the Quantum Hall effect. It is a two channel pump, where the two channels are connected by a loop of circumference l threaded by a slowly time-dependent magnetic flux Φ. The boundary condition at the vertices are such that at the Fermi energy the scattering at the vertices is a permutation matrix as shown in the Figure. Particles coming from the left are then forced to make a complete lap around the circle in clockwise sense, while particles coming from the right make a counter-clockwise U-turn. The pump is transmissionless and the reflection coefficients are phases, given



by a combination of the optical length of the loop and the Aharonov-Bohm phase

$$S(\mu, \Phi) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}(k_F l+\Phi)} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}(k_F l-\Phi)} \end{pmatrix},$$

what implies that the pump is optimal. The BPT formula gives then for the charge transport:

$$\langle dQ\rangle_{1,2} = \mp\frac{d\Phi}{2\pi}$$

A cycle of the pump is completed as the flux increases by a flux quantum 2π, producing a charge transport of 1. The scattering calculation is easy, but does not really explain how the pump works. The particle interpretation gives a clearer explanation of how the pump works: the changing of the flux creates an EMF around the loop, accelerating the particles moving counter-clockwise and decelerating the particles moving clockwise. In particular some slowly clockwise moving particles are turned around by the EMF, and

leave the pump to the left.

The U-turn pump is an highly schematic description of the Quantum Hall effect. In the Quantum Hall effect time reversal is broken by an external magnetic field. In the U-turn pump time reversal is broken by the permutation matrices associated with scattering at the vertices. In particular, the vertex condition may be implemented by the edge currents in the Quantum Hall effect in a Corbino disk [**66, 17**].

4.3. A calculation on the sphere. We now exemplify the geometric construction for the two channel case: if we write the scattering matrix in the form

$$S = \mathrm{e}^{\mathrm{i}\gamma} \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha}\cos\theta & \mathrm{e}^{-\mathrm{i}\varphi}\sin\theta \\ \mathrm{e}^{\mathrm{i}\varphi}\sin\theta & \mathrm{e}^{-\mathrm{i}\alpha}\cos\theta \end{pmatrix},$$

the first row of the scattering matrix is mapped to the point

$$\hat{n} = (\sin(\alpha+\varphi)\sin(2\theta), -\cos(\alpha+\varphi)\sin(2\theta), \cos(2\theta))$$

on the sphere.

The latitude on the sphere is determined by θ, and the combination $\alpha+\varphi$ determines the longitude. The changes in the fiber coordinates are determined by the equation of parallel transport, the BPT equation. Let the cycle of the pump, described by a loop ∂D in parameter space, happen with constant θ. After one complete cycle the scattering matrix returns to its initial value: $\Delta\alpha = 2\pi n$, $\Delta\varphi = 2\pi m$, and $\Delta\gamma = 0$. The charge transport is then

$$\langle dQ\rangle_1 = -n\cos^2\theta + m\sin^2\theta = (m+n)\sin^2\theta - n = -(m+n)\cos^2\theta + m\,,$$

where $2\sin^2\theta$ and $-2\cos^2\theta$ are the (signed) surfaces lying north (resp. south) with respect to the path $\pi(\partial D)$ on the sphere (in this paragraph we will commit the abuse of calling "surface" the actual surface divided by 4π). They determine the fractional part of the charge transport. The ambiguity of the choice of the region over which to integrate reflects in an ambiguity in the definition of the integer part of charge transport, related to the fact that the degree of the map is discontinuous across $\pi(\partial D)$, where the jump of the degree amounts to $m+n$. There is however no ambiguity of the interpretation if the loop is small, as the charge transport is almost quantized.

The excess dissipation is $(8\pi)^{-1}\sin^2(2\theta)(\dot{\alpha}+\dot{\varphi})$, it is proportional to the velocity square on the sphere. This confirms that, if the cycle is close to one pole, there is no ambiguity in splitting the charge transport into a (small) fractional part, and an optimal quantized part.

This allows to throw a closer look to the idealization we had in our discussion on the bicycle pump: the real bicycle pump is never completely transmissionless, as the valves have a finite height. The small transmission has then modulus $\sin\theta$, with $\theta \approx 0$ (the value of θ has small variations during the cycle, but this does not influence the

discussion given below). The cycle of the pump consists then of n small loops around the north pole, and the charge transport to the left is

$$\langle Q\rangle_1 = -n\cos^2\theta + 0 = -n + n\sin^2\theta\,,$$

In the first case the transport is seen as a big fractional quasi-quantized part, with no quantized transport. $-n\cos^2\theta$ is the area to the south of the path (as the path consists of n loops), and 0 is the degree of the map $\pi : D \to S^2$ evaluated at any point north of the path.

Reversing point of view one obtains the second equality: transport is given by a small fractional part, given by the (signed) area north to the loop, and an integer part, given by the degree of π evaluated at any point south to the loop, for instance the south pole, as in the interior of unit square in parameter space there are still n resonances of transmission.

The choice between the two is a matter of interpretation. In this case the physical interpretation favours the second, as the deviation from optimality is measured by the excess dissipation. In this sense, the optimal pump to which the bicycle pump is close transports n particles per cycle.

4.4. Classical scattering from a battery. This example shows that in the classical case the energy shift is not determined by time-independent scattering data. Consider the classical version of the battery, see Paragraph 2.1, with Hamiltonian function $H(x,p) = (1/2)(p-A)^2$, with gauge $A(x,t) = t\phi'(x)$ of compact support. Clearly the particle get accelerated from the battery. This is verified by noting that the function $f(x,p) = (1/2)(p-A)^2 + \phi(x)$ is a constant of motion, what is verified by the equation of motion $(d/dt)(p-A) = \dot{A} = \phi'$. In the leads $f = (1/2)p^2 + \phi$, hence the energy, defined there as $E = (1/2)p^2$, gets shifted by an amount $\mathcal{E} = \phi|_{-\infty}^{\infty}$. On the other hand, for the static scatterers $(p-A)$ is a constant of motion. As a consequence all the static scattering maps are equal to the identity map. This shows that the static scattering that cannot determine the energy shift, in contrast to the quantum case. The phase information available in the quantum case is of course not present in the classical one.

5. The theory of full counting statistics

We present now a short review of results of the theory of full counting statistics [**36, 35, 29, 2, 5**] for the quantities calculated above in the scattering formalisms. The object of study of the theory of full counting statistics is transport integrated over a full cycle, and this theory does not produce information which is local in time. On the other end, the noise can be calculated all the way down to $T = 0$, allowing therefore to verify that optimal pumps transport a quantized number of charges also in this regime. In the full counting statistics approach the results can be stated as identity rather that adiabatic approximations: the objects entering the description are the time-dependent

Hamiltonian $H(t)$, the Hamiltonian H_0 for the disconnected pump, the projection Q_j onto the j-th channel and the initial state ρ, which is assumed to be a thermal state $\rho(H_0)$. The assumptions about these objects are the following: $H(t)$ must equal H_0 in the distant past and the distant future and the projection Q_j must commute with the free Hamiltonian $[h_0, Q_j] = 0$.

The quantity describing transport in the full counting statistic approach is the generating function

$$\chi(\lambda) = \sum_{n\in\mathbb{Z}} p_n \mathrm{e}^{\mathrm{i}\lambda n}\,, \tag{3.48}$$

where p_n is the probability that n particles have been transferred to channel j during the entire process. The generating function allows to compute the moments $\langle Q_j^m\rangle$ and the cumulants $\langle\langle Q_j^m\rangle\rangle$ by differentiation

$$\langle Q^m\rangle_j = (\frac{1}{\mathrm{i}}\frac{d}{d\lambda})^m \chi(\lambda)|_{\lambda=0} \tag{3.49}$$

$$\langle\langle Q^m\rangle\rangle_j = (\frac{1}{\mathrm{i}}\frac{d}{d\lambda})^m \log(\chi(\lambda))|_{\lambda=0}\,. \tag{3.50}$$

It is given by the Lesovik-Levitov formula [**36**]

$$\chi(\lambda) = \det(1 + \rho(\mathrm{e}^{-\mathrm{i}\lambda Q_j/2}\mathrm{e}^{\mathrm{i}\lambda\hat{Q}_j}\mathrm{e}^{-\mathrm{i}\lambda Q_j/2} - 1)) \tag{3.51}$$

where $\hat{Q}_j = S_d^* Q_j S_d$, $\rho = \rho(H_0)$. The logarithm of the generating function is given, to second order in λ, as

$$\log\chi(\lambda) = \mathrm{i}\lambda\,\mathrm{Tr}(\rho A) - \frac{\lambda^2}{2}\,\mathrm{Tr}(\rho A(1-\rho)A) + O(\omega^3)\,,$$

where $A = \hat{Q}_j - Q_j$. This produces the following result for the first two cumulants, the charge transport and the noise:

$$\langle Q\rangle_j = \mathrm{Tr}(\rho A) = \mathrm{Tr}((\rho(H_0 - \mathcal{E}_d) - \rho(H_0))Q_j) \tag{3.52}$$

$$\langle\langle Q^2\rangle\rangle_j = -T\,\mathrm{Tr}(\rho' A^2) + \frac{1}{2}\,\mathrm{Tr}([\rho, A][A, \rho]) \tag{3.53}$$

The description of charge transport is clearly correct, as the right hand side of (3.52) is exactly what one means by charge transport. In the adiabatic limit it reduces therefore to the BPT formula. The two terms on the right hand side of (3.53), both positive, are the Johnson-Nyquist (thermal) noise, and the quantum shot noise. The first is proportional to temperature and vanishes for $T = 0$, the other involves correlations at different times and survives at $T = 0$. The quantum shot noise, as it is given in terms of commutators, vanishes in the semiclassical limit. We evaluate them with Weyl calculus analogously to the discussion (3.1), (3.2) and (3.4).

5.1. Thermal noise. The symbol corresponding to A is

$$\sigma(A) = S(E,t)^* P_j S(E,t) - P_j$$

where P_j is a matrix projecting onto the j-th channel. The Johnson-Nyquist noise at low temperature (where ρ' is concentrated near μ) is

$$2\pi \langle\langle Q_{JN}^2 \rangle\rangle = T \int_{-\infty}^{\infty} dt \, \mathrm{tr}(\sigma(A)^2(\mu,t)) = 2T \sum_{k \neq j} \int_{-\infty}^{\infty} dt |S|_{jk}^2(\mu,t) \,,$$

The integral is finite as for large times $H(t)$ coincides with H_0 and the scattering matrix is the identity matrix.

5.2. Shot noise at finite temperature. By repeated use of $[H_0, Q]$ we find

$$\langle Q_{SN}^2 \rangle = \frac{1}{2} \mathrm{Tr}([\rho, A][A, \rho]) = \frac{1}{2} \mathrm{Tr}([\delta\rho, Q][Q, \delta\rho]) \,.$$

The symbol associated to $[\delta\rho, Q]$ is (to leading order)

$$\sigma^{(SP)}([\delta\rho, Q]) = -\rho'(E)[\mathcal{E}(E,t), P_j] \,.$$

We have

$$\mathrm{tr}[\mathcal{E}(E,t), P_j][P_j, \mathcal{E}(E,t)] = 2((\mathcal{E}^2)_{jj} - (\mathcal{E}_{jj})^2) = 2\Delta\mathcal{E}_{jj}^2(E,t)$$

and we can legitimately multiply symbols, because at $T > 0$, $\rho'(E)$ is a smooth function. Evaluating the trace with (A.8) we obtain the result

$$\langle Q_{SN}^2 \rangle = \frac{\beta}{12\pi} \int dt \Delta_{jj}^2(\mu,t)$$

in agreement with the result obtained via adiabatic scattering.

5.3. Shot noise at $T = 0$. The result of the previous paragraph may lead one to believe that the noise diverges for $T = 0$. This is not the case: in the limit $T \to 0$ the symbols ρ', ρ'' are distributions, and it is not allowed to multiply them as we did in the previous paragraph. We can however write the quantum shot noise as

$$\langle Q_{SN}^2 \rangle = \frac{1}{2} \mathrm{Tr}([\rho, A][A, \rho]) = \mathrm{Tr}([\rho, \hat{Q}][\hat{Q}, \rho])$$

Approximating the symbol of $\hat{Q}$ by its value at the Fermi energy

$$\sigma(\hat{Q}_j) = S^*(E,t) P_j S(E,t) \approx S^*(\mu,t) P_j S(\mu,t) := p_j(t)$$

we approximate $\hat{Q}_j$ through a multiplication operator, therefore

$$\langle Q_{SN}^2 \rangle = \int\int dt dt' |\hat{\rho}(t-t')|^2 \, \mathrm{tr}(q_j(t) - q_j(t'))^2 \,,$$

where $\hat{\rho}$ is the Fourier transform of the Fermi function at $T = 0$

$$\hat{\rho}(t) = \frac{\mathrm{i}}{2\pi(t + \mathrm{i}0)} \mathrm{e}^{-\mathrm{i}t\mu} \,.$$

In the limit of large μ one obtains

$$\langle Q^2_{SN}(\mu)\rangle = \frac{1}{4\pi^2}\int\int dtdt' \frac{1-|S(\mu,t)S^*(\mu,t'))_{jj}|^2}{(t-t')^2}\,. \tag{3.54}$$

The integral is convergent: the integrand is bounded as the unitarity of S implies that the numerator vanishes at least quadratically for $t-t' \to 0$; the assumption that $H = H_0$ for large t implies that the integrand survives only on a narrow strip around the t and t' axis. This strips are in fact infinite, but the decay given by the denominator is sufficient to ensure convergence.

CHAPTER 4

Equivalence between topological and scattering approach to pumping

In this chapter we compare the topological and the scattering approach to quantum pumping, showing that the two descriptions are equivalent, as long as they are both applicable. This may seem surprising, because the idealization on which the two theories are based are quite different: in the topological approach a microscopic point of view is assumed, in the sense that the pump is modelled as an infinitely extended potential. Moreover the Fermi energy of the system is supposed to lie in a gap for all the time, and transport is attributed to states in the Fermi see at energies way below the Fermi energy. In the scattering approach the pump is viewed as a compact object, connected to gapless channels, where the particles move freely; and to calculate the charge transport the scattering matrix is evaluated at the Fermi energy only. In physical terms the first description applies to insulators, and the second to metals, or at least seemingly so.

It is however possible to compare the theories, constructing a compact pump by truncating the infinite potential of the topological approach to a finite interval and let the particles move freely in the two half lines appearing at the left respectively at the right of the truncation points. The systems becomes then amenable to the analysis of the scattering approach. In the limit where the pump is large, the truncated system approaches the original one, and one would want the predictions of the two theories to agree. This is in fact the case, as we will show in this chapter.

The equivalence was first established for the system originally considered by Thouless, i.e. a periodic one channel potential, and later extended to general n-channel potentials. We will present both these proves in Section 1 and Section 2 respectively, although the first is in fact implied by the second, and the guidelines of the proofs are somewhat similar. The reason for this redundancy is twofold: first, as the two proves are similar, the mechanism underlying the equivalence is already read out in the simpler case, where it is moreover less obscured by mathematical complications; second, as the strategic outline of the proofs is similar, the proof in the periodic case is perfectly suited to serve as an illustratory introduction in view of the general proof. For these reasons, the first proof is presented in a more informal way.

1. The 2 channel case

We begin by the simplest case: the comparison between the space and time periodic potential $V(x,t)$ of the topological approach and the pump obtained connecting two channels through a finite number of periods of $V(x,t)$, where the charge transport produced by the latter is given by the BPT formula (3.1). As the number of period grows large, one desires the two result to agree, and this is what we show in this section. The charge transport as expressed by the topological approach is the net number of zeroes of the (left unbounded) solution ψ_+ to the Schrödinger equation at the Fermi energy μ traversing a reference point x_0 in space. We recall the strategic elements of the proof of this fact, highlighted in Section 1: first, the Chern number (2.10) is calculated in a gauge which is defined everywhere except at singular points, and is therefore the sum of contributions of these singularities; second, the gauge is chosen in such a way that all the singularities, corresponding to nodes of ψ_+, lie on the circle $\{(z,s)|z=\mu,\ s\in S^1\}$; third, the sign of $\partial_z\psi_+$ at the singular points is related to the sign of the space derivative at the nodes, showing that the contribution of a singular point depends only on the direction in which the node traverses x_0 (in this section $x_0=0$).

To calculate the charge transport for the open pump, one starts by finding the frozen on-shell scattering matrix at the Fermi energy $S(\mu,t)$. If the number of period grows large, the tunnelling probability falls off exponentially, what means that the scattering matrix is transmissionless, and hence optimal, in the limit. In light of the discussion given in Section 3 we deduce the encouraging fact that the charge transport described by the scattering approach is quantized, being given by the winding number of the phase of r. The other encouraging fact is that the potential $V(x,t)$ enters the calculation of $S(\mu,t)$ only through ψ_+ and ψ_-, as is evident if the calculation is done in the standard textbook procedure of matching the plane waves solution in the channel to the general solution $A_+\psi_+ + A_-\psi_-$ in the pump. Of these, quite obviously, only ψ_+ will be relevant in the limit. Once that calculation is done, one is left with the easy task of determine the winding number of r.

Let us begin by the calculation of the scattering matrix: for a wave incident from the left the solution to the Schrödinger equation

$$H(s) = -\frac{d^2}{dx^2} + \chi_{[0,N]}(x)V(x,s)$$

is of the form

$$\begin{cases} \mathrm{e}^{\mathrm{i}px} + r_N\mathrm{e}^{-\mathrm{i}px} & , \quad (x\leq 0) \\ A_+\psi_+(x) + A_-\psi_-(x) & , \quad (0\leq x\leq N) \\ t_N\mathrm{e}^{\mathrm{i}px} & , \quad (x\geq NL) \end{cases}$$

with $p=\sqrt{\mu}$. Within the barrier the Wronskian of this solution and ψ_+ (or ψ_-) is constant, and in particular equal at $x=0$ and at $x=N$. The matching conditions thus

amount to

$$W(\mathrm{e}^{\mathrm{i}px} + r_N \mathrm{e}^{-\mathrm{i}px}, \psi_\pm)|_{x=0} = W(t_N \mathrm{e}^{\mathrm{i}px}, \psi_\pm)|_{x=N} \,.$$

Setting $W_\pm = W(\mathrm{e}^{\mathrm{i}px}, \psi_\pm)|_{x=0}$ and using

$$W(\mathrm{e}^{-\mathrm{i}px}, \psi_\pm)|_{x=0} = \overline{W}_\pm \,, \qquad W(\mathrm{e}^{\mathrm{i}px}, \psi_\pm)|_{x=N} = (-1)^{nN} \mathrm{e}^{\mp\kappa N} \mathrm{e}^{\mathrm{i}pN} W_\pm \,,$$

(what follows from

$$\psi_\pm(x+1) = (-1)^n \mathrm{e}^{\mp\kappa x} \psi_\pm(x)$$

with n giving the parity of the gap of the full $H(s)$) we find

$$r_N = -u_+ \frac{1 - \mathrm{e}^{-2\kappa N}}{1 - \mathrm{e}^{-2\kappa N} u_+ u_-^{-1}} \,,$$
$$t_N = (-1)^{nN} \mathrm{e}^{-\kappa N} \mathrm{e}^{-\mathrm{i}pN} \frac{1 - u_+ u_-^{-1}}{1 - \mathrm{e}^{-2\kappa N} u_+ u_-^{-1}}$$

with

$$u_\pm = \frac{W_\pm}{\overline{W}_\pm} = \frac{\psi'_\pm(0) - \mathrm{i}p\psi_\pm(0)}{\psi'_\pm(0) + \mathrm{i}p\psi_\pm(0)} \,. \tag{4.1}$$

Since $\psi_\pm$ is real, we have $|u_\pm| = 1$. Owing to the invariance of the Hamiltonian under time reversal, S is symmetric, i.e., $t'_N = t_N$. In the limit of a long barrier we have

$$r = \lim_{N\to\infty} r_N = -u_+ \,, \qquad t' = \lim_{N\to\infty} t'_N = 0 \,,$$

and the condition for optimality is attained exponentially fast in N. Restoring the dependence on s, the charge delivered to the left lead becomes

$$\lim_{N\to\infty} \langle Q_1 \rangle = \frac{\mathrm{i}}{2\pi} \int_{s=0}^{s=T} \left(\overline{r} dr + \overline{t}' dt' \right) = \frac{\mathrm{i}}{2\pi} \int_{s=0}^{s=T} \overline{u}_+ du_+ \,,$$

which, up to the sign, is the winding number of the phase $u_-(s)$. The charge crossing $x = 0$ in the positive direction is thus given by the winding number itself.

The winding number is obtained counting the (signed) passages of $u_+(s)$ through 1. The value 1 is attained when $\psi_+(0) = 0$, and whenever a node of $\psi_{+,s}$ crosses $x = 0$ from the left, $\partial_s \psi_+|_{x=0}$ and $\partial_x \psi_+|_{x=0}$ have opposite signs. Hence $u_+(s)$, which moves along the unit circle, see (4.1), crosses $u = 1$ from below, counting $+1$ to its winding number; nodes crossing $x = 0$ from the right contribute -1. This concludes the proof of the equivalence: the winding number describing the charge transport of the (optimal) truncated pump in the limit is the same as the Chern number describing the charge transported by the (infinite) potential in the topological approach.

2. 2n channels and non periodic potential

We will now prove the equivalence between the topological and the scattering approach to pumping in full generality. The comparison is analogous to the one given in the previous section: given a non-autonomous Hamiltonian

$$H(s) = \frac{d^2}{dx^2} + V(x,s)$$

as described in Chapter 2 (remember in particular that it has a periodic time dependence, and that the Fermi energy lies in a gap (2.2) for the entire process) we compare the following two systems. The first is the infinitely extended n channel lead subject to the potential $V(x,t)$, for which the charge transported to the right of a point x_0 (we from now on set $x_0 = 0$) (2.6) is (see Theorem 2)

$$\langle Q_T \rangle = \frac{\mathrm{i}}{2\pi} \oint_\gamma dz \oint_{S^1} ds \ \mathrm{tr}\big(W(\frac{\partial \tilde{\psi}_-}{\partial z}, \frac{\partial \psi_+}{\partial s}; 0) - W(\frac{\partial \tilde{\psi}_-}{\partial s}, \frac{\partial \psi_+}{\partial z}; 0)\big)\,.$$

The second is the one obtained connecting two n channel leads (represented by the half lines $x < 0$, $x > L$ respectively) through a finite (but eventually long) part of the potential V: $V_L(x,s) = V(x,s)\chi_{[0.L]}(x)$. The total charge emitted from the left lead is then given by the BPT formula as

$$\langle Q^{(L)}_{BPT} \rangle = \frac{1}{2\pi\mathrm{i}} \oint \mathrm{tr}((dS_L) S_L^* P)\,,$$

where $dS = (dS/ds)ds$ and $P = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ is the projection onto the n channels of the right lead. In the same situation the variance is [**29, 10**]

$$\langle\langle Q^2_{BPT} \rangle\rangle = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} ds \oint ds' \frac{\mathrm{tr}[(S_L^*(s) P S_L(s) - S_L^*(s') P S_L(s'))^2]}{\sin^2(s - s')}\,. \tag{4.2}$$

Because of (2.2) we expect the scattering matrix $S(\mu, s)$ (we drop μ in the following) to be transmissionless in the limit

$$S(s) = \begin{pmatrix} R(s) & 0 \\ 0 & R'(s) \end{pmatrix}\,,$$

(where R, R' are $n \times n$ matrices) and charge transport to be therefore quantized.

The equivalence in the two channel case obtained in the previous section provides us with a possible strategy to prove the main result of this Thesis, the equivalence between the two approaches, stated as

Theorem 4. *With the charge transports of the two theories defined as above the topological and the scattering approach agree in the limit of a long truncated pump:*

$$\langle Q_{BPT} \rangle := \lim_{L \to \infty} \langle Q^{(L)}_{BPT} \rangle = \langle Q_T \rangle\,. \tag{4.3}$$

For the proof of Theorem 4 we will therefore follow the same main steps as in the two channel case.

2.1. Choosing the gauge. In analogy with the two channel case, and in view of the right action (2.23), a section $\psi^0_+ : (z,s) \mapsto \psi^0_{(z,s)}(x)$ may be defined on all the torus by $\psi^0_{(z,s)}(0) = 1$, except for points (z_*, s_*) where the matrix $\psi_+(0)$ is singular. We need therefore to characterize these points: it is a consequence of Lemma 5 stated just below that any point $(z_*, s_*) \in \mathbb{T}$ where $\det \psi_+(0) = 0$ for some (and hence all) $\psi_+ \in S^+_{(z_*,s_*)}$ has z_* real and not below the spectrum of $H(s)$, whence $z_* = \mu$.

LEMMA 5. *Let $\psi_+ \in S^+_{(z,s)}$ and $x \in \mathbb{R}$. Then 0 is an eigenvalue of $\psi_+(x)$ iff z is a Dirichlet eigenvalue for $H(s)$ on $[x, \infty)$, including multiplicities. These conditions can occur only for $z \in \mathbb{R}$ and for isolated x.*

PROOF. Solutions $\varphi = \varphi(x)$ with values in $\mathbb{C}^n$ of the differential equation $H(s)\varphi = z\varphi$ are square-integrable at $x = +\infty$ iff $\varphi(x) = \psi_+(x)a$ for some $a \in \mathbb{C}^n$. Hence the equivalence of the two conditions. They imply $z \in \mathbb{R}$ because the operator $H(s)$ with Dirichlet boundary conditions on $[x, \infty)$ is self-adjoint. To show that x is isolated, we assume $x = 0$ without loss and Taylor expand $\psi_+(x)$ at $x = 0$ up to second order. Using (2.18) on the second derivative, we so obtain

$$\psi_+(x)^*\psi_+(x) = \\ P^\perp\big(\psi_+(0)^*\psi_+(0) + x(\psi'_+(0)^*\psi_+(0) + \psi_+(0)^*\psi'_+(0)) + x^2\psi_+(0)^*(V(0) - z)\psi_+(0)\big)P^\perp + \\ x^2\psi'_+(0)^*\psi'_+(0) + o(x^2)\,, \qquad (x \to 0)\,,$$

where an orthogonal projection $P^\perp = 1 - P$ onto $(\ker \psi_+(0))^\perp$ has been inserted for free as a result of $\psi_+(0)P = 0$ and of $\psi'_+(0)^*\psi_+(0) = \psi_+(0)^*\psi'_+(0)$, which follows from $W(\psi^*_+, \psi_+) = 0$, as ψ^*_+ is a solution of (2.21). For small $x \neq 0$ the two terms are positive semidefinite, with the first one being definite on $(\ker \psi_+(0))^\perp$. Since

$$\ker \psi_+(0) \cap \ker \psi'_+(0) = \{0\} \tag{4.4}$$

by (2.19), their sum is positive definite on all of $\mathbb{C}^n$. Hence $\psi_+(x)$ is regular. □

2.2. Movement of the nodes. We have identified the gauge we want to adopt for the calculation of the Chern number (2.25) and characterized the points where it is singular. The next step is to find a relation between the x and the energy derivative (evaluated at 0) of ψ_+ at a node, allowing to relate the contribution of the singularities to the "physical" motion of $\psi_+(x)|_{z=\mu}$ as s changes.

We assume in the following few paragraphs that the potential V is such that the following conditions hold:

(C1) The points s_* are isolated in S^1

(C2) 0 is a simple eigenvalue of $\psi_+(0)|_{(z=\mu, s=s_*)}$

(C3) $\det(\psi'_+(0))|_{(z=\mu,s=s_*)} \neq 0$.

We will eventually prove that these conditions hold for generic potentials, and extend the results we are going to prove with these assumptions to all potentials by continuity. The promised relation between ψ'_+ and $\partial_z\psi_+$ is the content of the following Lemma.

LEMMA 6. *Let $\psi_{(z,s)} \in S^+_{(z,s)}$ be a section defined in a neighbourhood in $\mathbb{C}\times S^1 \supset \mathbb{T}$ of any of the singular points $(z_* = \mu, s_*)$, which is analytic in z. Then the family of matrices $L(z,s) = \psi'_{(\bar z,s)}(x_0)^*\psi_{(z,s)}(x_0)$ has the reflection property*

$$L(z,s) = L(\bar z, s)^*\,. \tag{4.5}$$

Its eigenvalues are real for real z. There is a single eigenvalue branch $\lambda(z,s)$ vanishing to first order at (μ, s_*) with

$$\frac{\partial\lambda}{\partial z} < 0\,.$$

Its winding number there is therefore

$$w_{s_*} = -\operatorname{sgn}\big(\frac{\partial\lambda}{\partial z}\frac{\partial\lambda}{\partial s}\big)\Big|_{(z=\mu,s=s_*)} = \operatorname{sgn}\big(\frac{\partial\lambda}{\partial s}\big)\Big|_{(z=\mu,s=s_*)}\,.$$

PROOF. If $\psi_{(z,s)}(x)$ is a solution of (2.18), then $\psi_{(\bar z,s)}(x)^*$ is a solution of (2.21). Hence

$$L(\bar z,s)^* - L(z,s) = W(\psi^*_{(\bar z,s)}, \psi_{(z,s)}; 0) = 0,$$

by (2.36), proving the reflection property. The statement about the eigenvalue branch follows from (C2), (C3).

Let $u \in \mathbb{C}^n$ be the normalized eigenvector of $L(\mu, s_*)$ with eigenvalue $\lambda(\mu, s_*) = 0$. Then

$$\frac{\partial\lambda}{\partial z}\big|_{(\mu,s_*)} = \big(u, \frac{\partial L}{\partial z}\big|_{(\mu,s_*)}u\big) = \big(u,\, \psi'^*_+\frac{\partial\psi_+}{\partial z}u\big)\,, \tag{4.6}$$

since $\psi_+ u = 0$ at $(z=\mu, s=s_*)$. There we may write

$$\frac{\partial\lambda}{\partial z} = \big(u, (\psi^*_+{}'\frac{\partial\psi_+}{\partial z} - \psi^*_+\frac{\partial^2\psi_+}{\partial x\partial z})u\big) = -\big(u,\, W(\psi^*_+, \frac{\partial\psi_+}{\partial z}; x=0)u\big)\,.$$

On the other hand we have

$$W(\psi^*_+, \frac{\partial\psi_+}{\partial z}; x) = \int_x^\infty dx'\psi^*_+(z,x')\psi_+(z,x') > 0\,,$$

which follows by differentiating (2.22) w.r.t. x and by using (2.18)(see (2.13). The winding number can be read off from the linearisation

$$\lambda(z,s) = \frac{\partial\lambda}{\partial z}\Big|_{(\mu,s_*)}\cdot(z-\mu) + \frac{\partial\lambda}{\partial s}\Big|_{(\mu,s_*)}\cdot(s-s_*) + O(|z-\mu|^2 + |s-s_*|^2)\,,$$

where the derivatives are real. □

2.3. The Chern number. Having chosen a gauge the way we wanted, characterized its singular points and found the desired relation between $\psi'_+(0)$ and $\partial_z\psi_+(0)$ at these singular points we have set the stage for the calculation of the Chern number, what is achieved in the following Lemma.

LEMMA 7.

$$C = -\sum_{s_*} w_{s_*}\,.$$

PROOF. As announced above, the condition

$$\psi^0_{(z,s)}(0) = 1$$

defines a section ψ^0_+ of P on all of the torus except at points (z,s) where the matrix $\psi_+(z,s)$ is singular. We use it outside of the union $\cup_{s_*}U_{s_*}$ of arbitrarily small neighbourhoods of those points; inside we use a section $\hat\psi_+$ defined there. Using these local sections, the connection is expressed as a $\mathrm{gl}(n)$-valued one-form on the corresponding patches of the torus, e.g. $\psi^{0*}_+\mathcal{A}$ (with * exceptionally denoting the pull-back), and the trace of the curvature as a 2-form, $\operatorname{tr} D\mathcal{A} = d\operatorname{tr}\psi^{0*}_+\mathcal{A}$. Upon changing the patch we have $\hat\psi_+ = \psi^0_+ T$ with $T = T(z,s) \in \mathrm{GL}(n)$ and hence $\hat\psi^*_+\mathcal{A} = T^{-1}(\psi^{0*}_+\mathcal{A})T + T^{-1}(dT)$. So, using Stokes' theorem on (2.30), we express the Chern number as

$$C = \frac{\mathrm{i}}{2\pi}\sum_{s_*}\oint_{\partial U_{s_*}} \operatorname{tr}\hat\psi^*_+\mathcal{A} - \operatorname{tr}\psi^{0*}_+\mathcal{A} = \frac{\mathrm{i}}{2\pi}\oint_{\partial U_{s_*}} d\log\det T\,.$$

We may here replace $T = \hat\psi_{(z,s)}(0)\psi^0_{(z,s)}(0)^{-1} = \hat\psi_(z,s)(0)$ by $L(z,s)$, because of (C3). In U_{s_*} we have $L(z,s) = \lambda(z,s)P(z,s) + \tilde L(z,s)$, where $P(z,s)$ is a rank 1 projection and $\tilde L(z,s)$ is a regular linear map from $\ker P(z,s)$ to itself. Thus $\det L$ can be in turn replaced by $\det(\lambda P) = \lambda$ and the claim follows. □

2.4. Genericity of the assumptions. The next big step, if we want to maintain that we follow the strategy we learned in the two channel case, is the calculation of the frozen on-shell scattering matrix. Before doing this we prove the genericity of the assumptions (C1),(C2),(C3). We consider the class of potentials introduced in Chapter 2:

$$\mathcal{V} = \{V : \mathbb{R}\times S^1 \to M_n(\mathbb{C}) | V = V^*,\\ V(\cdot,s) \in L^\infty(\mathbb{R}, M_n(\mathbb{C})),\ \text{with}\ C^1\ \text{dependence on}\ s\in S^1\}\,.$$

The assumptions are generic in this class:

LEMMA 8. *The conditions (C1), (C2) and (C3) are satisfied by a dense set of potentials $V = V^*$.*

PROOF. If at (z_*, s_*) a matrix $\psi_+(0)$ is singular, that remains true under gauge transformations (2.23). Genericity of assumption (C1): Eigenvalue curves $f(s)$ of the Dirichlet Hamiltonian $H(s)$ on $[0,\infty)$ are continuously differentiable, even through crossings. By Sard's theorem the set $\{\mu' \in \mathbb{R} \mid f(s_*) = \mu', f'(s_*) = 0 \text{ for some } s_* \in S^1\}$ has zero measure. Upon adding to $V(x,s)$ an arbitrarily small constant we may assume that μ is not in that set. In particular, the points s_* are isolated, as claimed.

Genericity of assumptions (C2) & (C3): We further perturb V by $tW(x,s)$ where t is small and $W = W(x,s)$ is an arbitrary Hermitian matrix from the same class as V. To first order in t, the splitting of a degenerate Dirichlet eigenvalue μ of $H(s_*)$ is $\mu + t\tilde{\mu} + o(t^2)$, $(t \to 0)$, where the $\tilde{\mu}$ are obtained by solving the finite dimensional eigenvalue problem

(4.7)
$$P\Big(\int_0^\infty dx\, \psi_+(x)^* W(x,s_*)\psi_+(x)\Big)Pa = \tilde{\mu} P\Big(\int_0^\infty dx\, \psi_+(x)^*\psi_+(x)\Big)Pa\,, \qquad (a \in \mathbb{C}^n)\,,$$

and P is again the projection onto $\ker \psi_+(0)$. Since $\psi_+(x)$ is regular a.e., the matrix in brackets on the l.h.s. may take arbitrary Hermitian values, while that on the r.h.s. is positive definite on $\mathbb{C}^n$; the latter may then be set equal to 1 by means of a gauge transformation. As a result, the eigenvalues $\tilde{\mu}$ are generically distinct and, since $f'(s_*) \neq 0$, the points s_* split into non-degenerate ones. Moreover, points s_* with $\det \psi'_+(x_0) = 0$ correspond to Neumann eigenvalues. They are also perturbed and split according to (4.7), except that P now is the projection onto $\ker \psi'_+(0)$. Because of (4.4) the coincidence between Dirichlet and Neumann eigenvalues is generically lifted. □

2.5. Calculation of the scattering matrix. It is now time to evaluate the scattering matrix: the result is

LEMMA 9. *The scattering matrix $S_L(s)$ at Fermi energy μ has a limit of the form*

(4.8)
$$\lim_{L\to\infty} S_L(s) = \begin{pmatrix} R(s) & 0 \\ 0 & R'(s) \end{pmatrix}.$$

In particular, the variance (3.4) vanishes and quantization of $\langle Q_{BPT}\rangle$ is attained in the limit.

As a consequence the charge transport $\langle Q_{BPT}\rangle$ is an integer

$$\langle Q_{BPT}\rangle = \frac{1}{2\pi \mathrm{i}} \oint \mathrm{tr}((dU_1)U_1^*) = \frac{1}{2\pi \mathrm{i}} \oint d \log \det U_1\,,$$

given by the winding number of the determinant of R.

PROOF OF LEMMA 9. The scattering matrix $S_L = \left(\begin{smallmatrix} R_L & T'_L \\ T_L & R'_L \end{smallmatrix}\right)$ is that of the potential truncated to the interval $[0, L]$. The left incident solution of (2.18) is given by the

expression

$$\psi(x) = \begin{cases} 1\mathrm{e}^{\mathrm{i}kx} + R\mathrm{e}^{-\mathrm{i}kx}\,, & (x<0)\,, \\ T\mathrm{e}^{\mathrm{i}kx}\,, & (x>L)\,, \end{cases} \tag{4.9}$$

in the intervals $x \le 0$, resp. $x \ge L$. Its adjoint is a solution of (2.21) since $z = \mu$ is real. By the constancy of the Wronskian,

$$W(1\mathrm{e}^{-\mathrm{i}kx} + R_L^*\mathrm{e}^{\mathrm{i}kx}, \psi_\pm; x=0) = W(T_L^*\mathrm{e}^{-\mathrm{i}kx}, \psi_\pm; x=L)\,,$$

and by $W(1\mathrm{e}^{\mathrm{i}kx}, \psi_\pm; x) = \mathrm{e}^{\mathrm{i}kx}(\psi'_\pm(x) - \mathrm{i}k\psi_\pm(x))$ we find

$$\big(\psi'_\pm(0) + \mathrm{i}k\psi_\pm(0)\big) + R_L^*\big(\psi'_\pm(0) - \mathrm{i}k\psi_\pm(0)\big) = T_L^*\mathrm{e}^{-\mathrm{i}kL}\big(\psi'_\pm(L) + \mathrm{i}k\psi_\pm(L)\big)\,. \tag{4.10}$$

We have that

$$\lim_{x\to+\infty} \psi'_+(x) + \mathrm{i}k\psi_+(x) = 0\,, \tag{4.11}$$

$$\lim_{x\to+\infty} \big(\psi'_-(x) + \mathrm{i}k\psi_-(x)\big)^{-1} = 0\,. \tag{4.12}$$

Indeed, the first limit just repeats the definition (2.20) and the second may be rephrased to the effect that

$$A(x) := \big(\psi'_-(x) + \mathrm{i}k\psi_-(x)\big)^*\big(\psi'_-(x) + \mathrm{i}k\psi_-(x)\big)$$

is invertible with $\lim_{x\to+\infty} \|A(x)^{-1}\| = 0$. We note that

$$A(x) = \psi'_-(x)^*\psi'_-(x) + k^2\psi_-(x)^*\psi_-(x)\,,$$

since the cross term is $-\mathrm{i}kW(\psi_-^*, \psi_-) = 0$ by (2.36). If the claim were false, there would exist a sequence $x \to \infty$ and $a(x) \in \mathbb{C}^n$, ($\|a(x)\| = 1$) such that $\|\psi'_-(x)a(x)\| + \|\psi_-(x)a(x)\|$ remains bounded. Together with (4.11) this however contradicts the fact that $W(\psi_+^*, \psi_-)$ is regular. Having so established (4.12), we multiply the $-$ version of (4.10) by $\mathrm{e}^{\mathrm{i}kL}(\psi'_-(L) - \mathrm{i}k\psi_-(L))^{-1}$ from the right, while keeping the $+$ version unchanged. As $L \to +\infty$ the two equations then go over to

$$\begin{aligned} \big(\psi'_+(0) + \mathrm{i}k\psi_+(0)\big) + R^*\big(\psi'_+(0) - \mathrm{i}k\psi_+(0)\big) &= 0\,, \\ 0 &= T^*\,, \end{aligned} \tag{4.13}$$

in the sense that the coefficients do. Since the latter system has a unique solution (R^*, T^*), it is the limit of (R_L^*, T_L^*). □

2.6. Proof of the equivalence. We are now left with the task of relating the winding number of $\det R$ to the Chern number $\langle Q_T \rangle$, now reduced to $-\sum_{s_*} \mathrm{sgn}\big(\partial\lambda/\partial s\big)|_{(z=\mu, s=s_*)}$, task which is achieved by

Lemma 10. *The unitary matrix $R(s)$ has eigenvalue -1 iff $\det \psi_{\mu,s}(0) = 0$. More precisely, as s increases past s_*, an eigenvalue of R crosses -1 counterclockwise if*

$$\frac{\partial\lambda}{\partial s}\Big|_{(z=\mu, s=s^*)} < 0\,.$$

PROOF. The matrix R in (4.8) is determined by (4.13) or, after multiplication with R,

$$R\big(\psi'_+(0) + \mathrm{i}k\psi_+(0)\big) + \big(\psi'_+(0) - \mathrm{i}k\psi_+(0)\big) = 0\,.$$

This shows that $\psi_+(0)$ has eigenvalue 0 iff R has eigenvalue -1: $\psi_+(0)u = 0$ implies $(R+1)\psi'_+(0)u = 0$; conversely $(R+1)v = 0$ implies $R^*v = -v$ and then $\psi^*_+(0)v = 0$. Moreover

$$\dot{R}\big(\psi'_+(0) + \mathrm{i}k\psi_+(0)\big) + R\big(\dot{\psi}'_+(0) + \mathrm{i}k\dot{\psi}_+(0)\big) + \dot{\psi}'_+(0) - \mathrm{i}k\dot{\psi}_+(0) = 0\,. \tag{4.14}$$

We compute the rate at which the eigenvalue crosses -1 as

$$\dot{Z} = \frac{\big(\psi'_+(0)u,\, \dot{R}\psi'_+(0)u\big)}{\big(\psi'_+(0)u,\, \psi'_+(0)u\big)}\,,$$

since the eigenprojection of the unitary R is orthogonal. Multiplying (4.14) with $\psi'_+(0)u$ from the left and with u from the right we obtain, using $R^*\psi'_+(0)u = -\psi'_+(0)u$,

$$\big(\psi'_+(0)u,\, \dot{R}\psi'_+(0)u\big) - 2\mathrm{i}k\big(\psi'_+(0)u,\, \dot{\psi}_+(0)u\big) = 0$$

and hence

$$\dot{Z}\,\big(\psi'_+(0)u,\, \psi'_+(0)u\big) = 2\mathrm{i}k\frac{\partial\lambda}{\partial s}\,.$$

□

The proof of Theorem 4 now follows easily.

PROOF OF THEOREM 4. It follows from Lemma 10 that $\langle Q_T\rangle$ is the (net) number of eigenvalues of $R(s)$ going through -1, i.e. the winding number of R. This proves the Theorem for all potentials V is such that the conditions (C$_i$), $i = 1, 2, 3$ are satisfied. Such potentials form a dense set, by Lemma 8, and the difference $\langle Q_T\rangle - \langle Q_{BPT}\rangle$ has a continuous dependence on the potential V. The equality extends therefore to all $V \in \mathcal{V}$ by continuity. ■

APPENDIX A

The Weyl calculus

Here we give a short description of the Weyl calculus [**53, 38**] to the extent that is needed to understand the derivations given in Paragraph 2.2.

Weyl calculus is a procedure particularly useful in semiclassical analysis and quantum statistical mechanics. It bases on a quantization procedure, by what one means a procedure to assign to classical observables f (i.e. (in our case matrix valued) functions on classical phase space) operators on Hilbert space $\mathrm{Op}_W(f)$ representing the analogous quantum observable, respecting the assignment

$$E \leftrightarrow E : \psi \mapsto E\psi$$
$$t \leftrightarrow -\mathrm{i}\omega\partial_E : \psi \mapsto -\mathrm{i}\psi'$$

and the condition of reality $\mathrm{Op}_W(f^*) = \mathrm{Op}_W(f)^*$. The Weyl quantization is singled out by the property

$$\mathrm{e}^{-\mathrm{i}L(E,-\mathrm{i}\omega\partial_E)}\mathrm{Op}_W(f) = \mathrm{Op}_W(\mathrm{e}^{-\mathrm{i}L(E,t)}f)\,,$$

for $L(E,t)$ any linear function, and is given by

$$\langle E,j|\mathrm{Op}_W(f)|\psi\rangle = \frac{1}{2\pi}\int\int dtdE' \sum_{l=1}^{n} \mathrm{e}^{-\mathrm{i}(E-E')t} a_{jl}(\frac{E+E'}{2},\omega t)\psi_l(E') \tag{A.1}$$

(to give a precise mathematical sense to the integral (A.1) one need to do some work [**53**], as the integrand is normally not absolutely convergent, and one has to exploit the strong oscillations of the phase).

In the semiclassical limit one is interested in the reverse direction of assignment $\sigma = \mathrm{Op}_W^{-1}$: a symbol $\sigma_{jj'}(A)$ corresponds to an operator A if and only if

$$\langle E,j|A|E',j'\rangle = \frac{1}{2\pi}\int dt \mathrm{e}^{\mathrm{i}(E-E')t}\sigma_{jj'}(A)(\frac{E+E'}{2},\omega t)\,, \tag{A.2}$$

or, equivalently,

$$\langle t,j|A|t',j'\rangle = \frac{1}{2\pi}\int dt \mathrm{e}^{-\mathrm{i}(t-t')E}\sigma_{jj'}(A)(E,\omega\frac{t+t'}{2})\,. \tag{A.3}$$

Given an operator A, one would then express the symbol $\sigma_{jj'}(A)$ as a (formal) power series in ω

$$\sigma_{jj'}(A) = \sum_n \omega^n \sigma^{(n)}_{jj'}(A)\,,$$

formal meaning that the series need not to converge, but the truncated (to $n = N$) series approximates the symbol to order ω^{N+1}. The first two terms in the expansion are called

$$\begin{aligned} \sigma^{(0)}_{jj'}(A) &=: \sigma^{(P)}_{jj'}(A) && \text{principal symbol} \\ \sigma^{(1)}_{jj'}(A) &=: \sigma^{(SP)}_{jj'}(A) && \text{subprincipal symbol}\,. \end{aligned}$$

In Chapter 4 we write $\sigma_{jj'}(A)(E, \omega t)$ as $\sigma_{jj'}(A)(E, t)$, although we state that the "real" dependence of the symbols is through ωt (where by real we mean producing an $O(\omega^0)$ derivative), what has as a consequence that the expansion does not display the power dependence on ω explicitly, absorbing it in the single terms.

Obviously, the assignment operator-symbol cannot conserve the product, as the product of one channel symbols is commutative and the product of operators is not. Clearly, one can nevertheless describe the symbol of the product $\sigma_{jj'}(AB)$ in terms of the symbols of the factors $\sigma_{jj'}(A)$, $\sigma_{jj'}(B)$. For the principal and subprincipal symbol one gets

$$\sigma^{(P)}(AB) = \sigma^{(P)}(A)\sigma^{(P)}(B) \tag{A.4}$$

$$\sigma^{(SP)}(AB) = \sigma^{(P)}(A)\sigma^{(SP)}(B) + \sigma^{(SP)}(A)\sigma^{(P)}(B) + \frac{1}{2\mathrm{i}}\{\sigma^{(P)}(A), \sigma^{(P)}(B)\}\,, \tag{A.5}$$

where the multiplication between the symbols is matrix multiplication and with $\{a, b\}_{jl} = \sum_k \{a_{jk}, b_{kl}\}$ denoting the Poisson bracket. In particular the subprincipal symbol of the commutator is

$$\sigma^{(SP)}([A, B]) = \{\sigma^{(P)}(A), \sigma^{(P)}(B)\}\,. \tag{A.6}$$

For a function ρ of the operator A one finds the symbol

$$\begin{aligned} \sigma(\rho(A)) = {} & \rho(\sigma^{(P)}(A)) \\ & + \omega\rho'(\sigma^{(P)}(A))\,\sigma^{(SP)}(A) \\ & + \omega^2\big(\rho'(\sigma^{(P)}(A))\sigma^{(2)}(A) + \frac{1}{2}\rho''(\sigma^{(P)}(A))\sigma^{(SP)}(A)^2 + R\big) + O(\omega^3)\,, \end{aligned} \tag{A.7}$$

where

$$\begin{aligned} R = {} & \rho''(\sigma^{(P)}(A))\big(\frac{1}{8}\mathrm{i}\partial_E\partial_\omega\sigma^{(P)}(A) - \frac{1}{16}\partial_E^2\sigma^{(P)}(A)\partial_t^2\sigma^{(P)}(A) \\ & - \rho'''(\sigma^{(P)}(A))\Big(\frac{1}{12}\mathrm{i}\partial_E\sigma^{(P)}(A)\partial_t\sigma^{(P)}(A) \\ & - \frac{1}{48}\big(\partial_t^2\sigma^{(P)}(A)(\partial_E\sigma^{(P)}(A))^2 + \partial_E^2\sigma^{(P)}(A)(\partial_t\sigma^{(P)}(A))^2\big)\Big)\,. \end{aligned}$$

The Weyl calculus is a precious tool in quantum statistical mechanics as it allows to calculate the expectation value of an operator A in the state ρ, previous knowledge of the corresponding symbols, as an integral over phase space. In fact for a trace class

operator A one has

$$\mathrm{Tr}(A) = \frac{1}{2\pi} \int \mathrm{tr}(\sigma(A)) dE dt \,, \tag{A.8}$$

and for the expectation value it holds

$$\mathrm{Tr}(\rho A) = \frac{1}{2} \int \mathrm{tr}(\sigma(\rho)\sigma(A)) dE dt \,. \tag{A.9}$$

APPENDIX B

Classical currents,semiclassical currents, and $\mathcal{T}$-$\mathcal{E}$ uncertainty

In This appendix we provide with a proof of (3.24) that will set the stage on a derivation of the BPT formula highlighting the role played by the energy shift-time delay uncertainty in transport [**10**].

1. The classical case

We start the proof of (3.24) observing that the charge transported in the time interval $[0, T]$ is

$$Q_j = \int_{\Gamma_j} dE'dt\chi_{[0,T]}(t)\rho(E) - \int_{\Gamma_j} dEdt\chi_{[0,T]}\rho(E)\,. \tag{B.1}$$

where in the first integral E is given through the scattering map (3.22). A point of precision has to be made, because of the non bijectivity of the scattering map: if $(E', t', j) \in \Gamma/\Gamma_+$, what may occur for $E' > 0$ small, i.e. close to the threshold energy 0 and $E < 0$, we assume that $g(E) = g(0)$, i.e. the occupations at the bound state and at the threshold are the same.

The formula (3.24) is immediately recovered substituting ρ in the first integral with its linear approximation, valid to order ω. We give another proof, which gives more space to physical interpretation: the first integral is rewritten as

$$\int_{\Gamma_j} dE'dt'\chi_[0,T](t)g(E) - \int_0^\infty dE'g(E)\mathcal{T}|_{t=0}^{t=T}\,. \tag{B.2}$$

To calculate the first integral we exploit the fact that Γ_j is described to lowest approximation by $\cup_j\Gamma_{ij}$, where Γ_{ij} is composed of states (E', t', j) originated from channel i through static scattering. Their preimages (E, t, i) appearing as arguments in the integral, are shifted with respect to them by the vectorfield $-(\mathcal{E}, \mathcal{T})$, to next approximation. The vectorfield is divergencefree, by (3.23), so that the difference between the first integral in (B.2) and the second integral in (B.1) reduces to the contributions given by discontinuities at the boundaries $\partial\Gamma_{ij}$. We divide these boundaries between the $E = 0$ part of it, and inner boundaries. The contribution of the first is

$$\int dt\mathcal{E}(0, t, j)\,,$$

and we write the contribution of the latter as

$$\int_{\Gamma_j} dEdtg(E)\Omega_j(E, t)\,,$$

where Ω_j is a distribution supported on the inner boundaries. Since the scattering map is bijective, the displacements of the Γ_{ij} are such that $\sum_j^n \Omega_j(E,t) = 0$.

The charge transport (B.1) is then

$$Q_j = \int_0^T dt\mathcal{E}(0,t,j) - \int_0^\infty dEg(E)\mathcal{T}(E,t,j)|_{t=0}^{t=T} + \int_0^\infty dE \int_0^T dtg(E)\Omega(E,t,j)$$

generating a current

$$\dot{Q}_j = \mathcal{E}(0,t,j) - \int_0^\infty dEg(E)\dot{\mathcal{T}}(E,t,j) + \int_0^\infty dEg(E)\Omega(E,t,j). \tag{B.3}$$

The three terms in (B.3) have a clear physical interpretation: the first term describes the releasing and trapping of particles from the pump; the second term describes the change of the flow caused by the change in the time delay, as an increase of $d\mathcal{T}$ cause no particle to exit the pump for $dt = d\mathcal{T}$; and the third term describes the transport from one channel to the other, with no withholdings as $\sum_j \Omega_j = 0$.

By evaluating the two last integrals, (3.24) is recovered. Divide the energy axis in the intervals over which the scattering map is continuous $[E_l, E_{l+1}[$, and denote by $\Delta\mathcal{E}_l$, $\Delta\mathcal{T}_l$ the discontinuities of $\mathcal{E}$, $\mathcal{T}$ across the points E_i: $\Delta\mathcal{E}_l = \mathcal{E}(E_l+,t,j) - \mathcal{E}(E_l-,t,j)$ and $\Delta\mathcal{T}$ the same way. The third integral in (B.3) is then

$$\sum_l (\Delta\mathcal{E}_l - \dot{E}_l\Delta\mathcal{T}_l)g(E_l)\,, \tag{B.4}$$

and the second

$$+\sum \dot{E}_l\Delta\mathcal{T}_l g(E_l) + \sum_l \int_{E_{l-1}}^{E_l} g(E)\mathcal{E}'(E,t,j) \tag{B.5}$$

where we also used (3.23). Integrating by parts the last term in (B.5) one obtains

$$-\sum_l \int_{E_{l-1}}^{E_l} g'(E)\mathcal{E}(E,t,j) - \mathcal{E}(0,t,j) - \sum_l \Delta\mathcal{E}_l g(E_l)\,. \tag{B.6}$$

The sums in (B.5) and (B.6) cancel against the one in (B.4), and the $\mathcal{E}(0,t,j)$ in (B.6) cancel against the one in (B.3), so that (3.24) is recovered.

2. Semiclassical currents

In this section we will give a semiclassical derivation of the BPT formula that relates currents to the uncertainty

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

in time delay-energy shift. This derivation will formally go through the same lines as the classical one, and will in particular display a formula admitting the same physical interpretations as (B.3). Analysing incoming wave packets whose center has trajectory $-x = \epsilon'(k_0)t + c$, one finds that the average time delay for outgoing particles in channel j is the diagonal element of the matrix of time delay $\mathcal{T}_{jj}$. With this, and with the

interpretation of the energy shift (3.18) given above, the semiclassical formula for the charge transported in the time interval $[0, T]$ is

$$\langle Q_j \rangle = \frac{1}{2\pi} \int_0^\infty dE' \int_0^T dt' \rho(E) - \frac{1}{2\pi} \int_0^\infty dE \int_0^T dt \rho(E)$$

(in a semiclassical context $g = \rho/2\pi$) where E in the first integral is given through the map

$$\Phi : (E', t') \mapsto (E, t) = (E' - \mathcal{E}_{jj}(E', t'), t' - \mathcal{T}_{jj}(E't')) .$$

The BPT formula is obtained approximating $\rho(E)$ linearly in the first integral and integrating by parts.

Another possible derivation is using Φ as a change of variables: the Jacobian of Φ is $1 - \Omega_{jj}$, where Ω_{jj} is the divergence of the displacement $(\mathcal{E}_{jj}, \mathcal{T}_{jj})$ and is the jj-th matrix element of the time delay-energy shift uncertainty

$$\Omega = \mathrm{i}[\mathcal{T}, \mathcal{E}] = \mathcal{E}' + \dot{\mathcal{T}} . \tag{B.7}$$

The map is invertible, as Ω_{jj} is of order ω and hence the Jacobian of order 1. After the change of variables, the first integral extends over $\Phi([0, \infty] \times [0, T])$, and the difference between the two is given by

$$\langle Q_j \rangle = - \int_0^\infty dE \rho(E) \mathcal{T}_{jj}(E, t)|_0^T - \int_0^T dt \rho(E) \mathcal{E}_{jj}(E, t)|_0^\infty + \int_0^\infty dE \int_0^T dt \rho(E) \Omega_{jj}(E, t) ,$$

and the current by

$$\langle \dot{Q}_j \rangle = \rho(0) \mathcal{E}_{jj}(E, t) - \int_0^\infty dE \rho(E) \dot{\mathcal{T}}_{jj}(E, t) - \int_0^\infty dE \Omega_{jj}(E, t) . \tag{B.8}$$

The terms in (B.8) admit the same interpretation as in the classical case: the first term describes the freeing and trapping of particles from the pump, and is constituted by Dirac delta term when the pump admits a semibound state [**10**] (i.e. a state that can be turned either in a bound state or in a scattering state by an arbitrarily small perturbation); the second term describes the change of the flux of particle as a consequence of the variation of the average time delay; and the third term describes transfer from one channel to another.

Inserting (B.7) into (B.8), the BPT formula is one partial integration away.

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Curriculum Vitae.

Personal

Gregorio Ortelli
Nussbaumstrasse 6
8003 Zürich
Switzerland

Born April 14, 1981 in Locarno
Swiss citizen

Education

Oct. 05 - Oct 09:	Doctoral studies in mathematical physics, Inst. Theoretical Physics, ETHZ, Zürich;
Oct. 00 - Aug. 05:	Master of science in physics, ETH, Zürich, including:
May 05 - Aug. 05:	Master project, Inst. Theoretical Physics, ETHZ, Zürich; under the supervision of Prof. Dr. Gian Michele Graf;
Sep. 96 - Jun. 00:	Maturità federale tipo B, Liceo Diocesano Breganzona

Academic teaching experience

Sept. 05 - May 09:	ETHZ teaching assistant: quantum mechanics, thermodynamics, electrodynamics, general relativity, quantum field theory;
Oct. 01- Jun. 05:	tutoring at ETHZ: analysis, linear algebra.

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