# Thinking transport as a twist 

Cristian Giardinà *<br>Jorge Kurchan ${ }^{\dagger}$

July 18, 2008


#### Abstract

The determination of the conductivity of a deterministic or stochastic classical system coupled to reservoirs at its ends can in general be mapped onto the problem of computing the stiffness (the 'energy' cost of twisting the boundaries) of a quantum-like operator. The nature of the coupling to the reservoirs determines the details of the mechanical coupling of the torque at the ends.


## 1 Introduction

The transport properties of a physical systems reserve many surprises, particularly in low dimensions, and despite many decades of efforts, a general theory is surprisingly not yet available [1, 2]. This is true even at the classical level.

The conductivity of low dimensional systems is often anomalous: the transport coefficients diverge with the system size. In such cases, the nature of the contact with the reservoirs at the boundaries becomes an issue. For example, the thermal conductivity of a finite chain becomes zero not only in the obvious case in which the contact is bad, but also in the limit when it is too good [2, 3]. A conductivity computed on the basis of a closed chain without reservoirs can clearly not take into account these effects. In any concrete physical realization of transport with anomalous properties, one hence has to consider the system as composed of both the bulk and the bath.

Spin and charge currents in closed quantum chains have been related to the corresponding stiffnesses [4, 5]. This relation between a transport and an equilibrium property has been very fruitful. More recently, the question of a quantum open chain without baths has been addressed [6].

[^0]In this paper we follow a different path. We shall establish a general correspondence between $i$ ) the transport properties of any classical (stochastic or deterministic) system in contact with reservoirs at its boundary, and ii) the stiffness (or helicity modulus [7]) of a zero-temperature system that is perturbed at the ends by a twist applied through two elastic 'handles' (see Figure 1). In this mapping, the details of the coupling between these handles and the system are important and reflect the nature of the coupling between reservoirs and the lattice in the original setting.

As we shall see, the correspondence we discuss here works at a different level from the one of Kohn [4] and Shastry-Sutherland [5]. Here, the stiffness one calculates is that of the evolution operator [8] and not of the energy itself 14 .

The plan of the paper is the following. In the next section we introduce our setting, recall the definition of conductivity and of stiffness and explain our strategy. We will find convenient to use the operator bra-ket notation by which the probability distribution of Eq. (11) is associated to a Hilbert space quantum-like "state"; this is described in Section 3, together with two examples that will be repeatedly used in the paper. Armed with this preliminaries, we first show in Section 4 that the bulk current in a transport model subject to a gradient in the boundary conditions can be expressed in terms of a 'helical' operator. We then use linear response theory to rederive in Section 5 two equivalent expressions of the finite volume conductivity: the first coincides with the standard Green-Kubo formula (i.e., time integral of the bulk current autocorrelation function); the second one involves the autocorrelation function of an operator which depends only on the boundaries. This second expression allows us to show that the conductivity is proportional to the stiffness of the evolution operator when a twist is exerted at the boundaries. This is shown in Section 6, which is then followed by conclusions.

## 2 Transport model

Consider an extended system made of $N$ components whose temporal evolution is either deterministic (Hamiltonian) or stochastic and whose boundaries are coupled to reservoirs. A convenient description of the system is given by the evolution (Fokker-Planck, Liouville,...) equation

$$
\begin{align*}
\frac{\partial}{\partial t} \mu(x, t) & =-H \mu(x, t) \\
\mu(x, t) & =e^{-t H} \mu(x, t=0) \tag{1}
\end{align*}
$$

where

- $\mu(x, t)$ is the probability distribution in a point $x$ of the phase/configurations space at time $t$.

[^1]

Figure 1: Stiffness of a bar twisted by elastic handles.

- $H$ is the evolution operator which is assumed of the form

$$
\begin{equation*}
H=H_{B}+\lambda\left(H_{L}\left(\alpha_{L}\right)+H_{R}\left(\alpha_{R}\right)\right) \tag{2}
\end{equation*}
$$

Here $H_{B}$ denotes the bulk evolution, whereas $H_{L}\left(\alpha_{L}\right)$ and $H_{R}\left(\alpha_{R}\right)$, which depend on a parameter $\alpha$, describe the interaction with reservoirs connected at the left/right boundaries, respectively. We have made explicit the strength of the coupling to the reservoirs with the parameter $\lambda$.

### 2.1 Conductivity

We consider situations when the bulk evolution has a constant of motion $E(x)$ typically the energy or the mass. We shall assume $E(x)$ is spatially local: it is the sum of N local contributions

$$
\begin{equation*}
E=\sum_{i=1}^{N} E_{i} \tag{3}
\end{equation*}
$$

each $E_{i}$ a function of the site $i$ or its near-neighbors.
Because the expectation of $E$ for an isolated system evolving through $H_{B}$ satisfies:

$$
\begin{equation*}
\frac{d}{d t}\langle E\rangle=\frac{d}{d t} \int d x E(x) \mu(x, t)=-\int d x\left[E, H_{B}\right] \mu(x, t)=0 \quad \forall \mu(x, t) ; \tag{4}
\end{equation*}
$$

this implies that $E$ commutes with the bulk evolution operator:

$$
\begin{equation*}
\left[E, H_{B}\right]=0 \tag{5}
\end{equation*}
$$

The reservoirs violate the conservation of $E$

$$
\begin{equation*}
\left[E, H_{L}\right] \neq 0 \quad ; \quad\left[E, H_{R}\right] \neq 0 \tag{6}
\end{equation*}
$$

and, in addition, if the values of the parameter $\alpha_{L} \neq \alpha_{R}$ are different, a current is established, a stationary state eventually sets in and one has transport of the quantity $E$ from one boundary to the other. Examples are:

- when the parameter is the temperature, $\alpha=T$, one has transport of energy;
- when the parameter is a particle density, $\alpha=\rho$, one has transport of mass.

If $\alpha_{R}-\alpha_{L}$ is small, in the stationary regime the averaged total current across all links $\langle\mathcal{J}\rangle$ is linear:

$$
\begin{equation*}
\langle\mathcal{J}\rangle \sim \kappa_{N}\left(\alpha_{R}-\alpha_{L}\right) \tag{7}
\end{equation*}
$$

which defines the conductivity $\kappa_{N}$ for a system of size $N$.

### 2.2 Stiffness

In order to recall the definition of the stiffness let us consider a simple example which is totally independent from the context of transport models. Suppose we are given a quantum Hamiltonian

$$
\begin{equation*}
\bar{H}=\bar{H}_{B}+\lambda\left(\bar{H}_{L}+\bar{H}_{R}\right) \tag{8}
\end{equation*}
$$

with a bulk part

$$
\begin{equation*}
\bar{H}_{B}=-\sum_{i=1}^{N} \hbar^{2} \frac{\partial^{2}}{\partial x_{i}^{2}}-\sum_{i=1}^{N-1} \cos \left(x_{i+1}-x_{i}\right) \tag{9}
\end{equation*}
$$

which clearly has symmetry with respect to simultaneous shift of all angles. The expectation of the global angle is fixed by two boundary terms:

$$
\begin{equation*}
\bar{H}_{L}=-\cos \left(x_{1}\right) \quad ; \quad \bar{H}_{R}=-\cos \left(x_{N}\right) \tag{10}
\end{equation*}
$$

which impose an optimal average profile $\left\langle x_{i}\right\rangle=0$ for all $i \in\{1, \ldots, N\}$. If we wish to calculate the stiffness, taking into account the specific coupling, we do the following: we compute first the lowest eigenvalue $\epsilon^{o}$ of $\bar{H}_{B}+\lambda\left(\bar{H}_{L}+\bar{H}_{R}\right)$. Next, we twist the two 'handles'

$$
\begin{equation*}
\bar{H}_{L}^{\mathrm{twisted}}=-\cos \left(x_{1}+\theta\right) \quad ; \quad \bar{H}_{R}^{\mathrm{twisted}}=-\cos \left(x_{N}-\theta\right) \tag{11}
\end{equation*}
$$

and calculate the new lowest eigenvalue $\epsilon^{\theta}$. In the limit where the coupling $\lambda \rightarrow 0$ then, of course, imposing the twist has no effect. In the opposite limit $\lambda \rightarrow \infty$ then $x_{1}=-\theta$ and $x_{N}=\theta$ are strictly imposed. For a finite value of the coupling $0<\lambda<\infty$ there is a competition between the bulk lattice which prefers a flat profile and the boundaries which force a gradient. In the framework of elasticity theory, the stiffness $\sigma_{N}$ measures the cost of twisting and is defined from

$$
\begin{equation*}
\epsilon^{\theta}-\epsilon^{o} \sim \frac{1}{2} \frac{\sigma_{N}}{(N-1)}(2 \theta)^{2} \tag{12}
\end{equation*}
$$

valid to first order in $\theta^{2}$. The factor $N-1$ assures a good scaling for large $N$ in a system with normal elasticity.

To define the stiffness of the transport model, which includes bulk and reservoirs, we proceed in a similar manner. We think of the evolution operator $H$ in formula
(11) as a quantum-like, albeit non-Hermitian, Hamiltonian. We can interpret (5) as an invariance of the bulk with respect to 'rotations' of angle $\theta$ generated by a group $e^{i \theta E}$.

The boundary couplings break this invariance (cfr. (6)), we can use them as 'handles' to impose a 'twist' by applying the transformation in opposite directions at the ends:

$$
\begin{equation*}
H_{R}^{\mathrm{twisted}}=e^{i \theta E} H_{R} e^{-i \theta E} \quad ; \quad H_{L}^{\mathrm{twisted}}=e^{-i \theta E} H_{L} e^{i \theta E} \tag{13}
\end{equation*}
$$

The (zero-temperature) stiffness $\sigma$ of the handle+bulk system is defined as in (12) from the increase in the lowest eigenvalue of $H^{\text {twisted }}(\theta)=H_{R}^{\mathrm{twisted}}+H_{B}+H_{L}^{\mathrm{twisted}}$ for small $\theta$.

The results we shall show in what follows is that the conductivity $\kappa$ is, up to a trivial factor, equal to the stiffness $\sigma$. In general, anomalous conductivity amounts to the system becoming rigid, due to long-range correlations. When the coupling to the bath is weak, the conductivity is small: the stiffness is also weak because the handles turn without affecting the system. In the opposite case, when the coupling is too strong, the conductivity of a system with anomalous diffusion may go to zero. From the point of view of elasticity, what happens is that the handles twist strongly the first and last sites of the chain, and it is more favorable for a stiff system to concentrate all the twist between the first two (and between the last two) sites.

## 3 Bracket Notation

A convenient way to write the evolution equation (11) is provided by the bra-ket formalism. The probability distribution at time $t$ is encoded in the state $|\psi(t)\rangle$, namely

$$
\begin{equation*}
|\psi(t)\rangle=\int d x \mu(x, t)|x\rangle \tag{14}
\end{equation*}
$$

where $|x\rangle$ denotes a vector which together with its transposed $\langle x|$ form a complete basis of a Hilbert space and its dual, that is

$$
\begin{equation*}
\left\langle x \mid x^{\prime}\right\rangle=\delta\left(x-x^{\prime}\right) \tag{15}
\end{equation*}
$$

It immediately follows that

$$
\begin{equation*}
\langle x \mid \psi(t)\rangle=\mu(x, t) \tag{16}
\end{equation*}
$$

and the evolution equation (11) takes the form of a Schrödinger equation with imaginary time

$$
\begin{equation*}
\frac{d}{d t}|\psi(t)\rangle=-H|\psi(t)\rangle \tag{17}
\end{equation*}
$$

To compute expectation we introduce the flat state

$$
\begin{equation*}
\langle-|=\int d x\langle x| \tag{18}
\end{equation*}
$$

which is such that

$$
\begin{equation*}
\langle-\mid x\rangle=1 \tag{19}
\end{equation*}
$$

Then for any observable $A$ we have that its expectation value at time $t$ can be written as

$$
\begin{equation*}
\langle A(t)\rangle=\int d x \mu(x, t) A(x)=\langle-| A|\psi(t)\rangle \tag{20}
\end{equation*}
$$

Conservation of probability implies that

$$
\begin{equation*}
\langle-| H=0 . \tag{21}
\end{equation*}
$$

The stationary state $|\psi\rangle$ satisfies

$$
\begin{equation*}
H|\psi\rangle=0 \tag{22}
\end{equation*}
$$

For an isolated system, namely $\lambda=0$, the invariant measure are given by any arbitrary function of $E$, as it is immediately seen from Eq.(5). For example the microcanonical ensemble is given by the uniform measure

$$
\begin{equation*}
|\psi\rangle_{e}=\int d x \delta(E(x)-N e)|x\rangle \tag{23}
\end{equation*}
$$

In the presence of reservoirs, namely $\lambda \neq 0$, the stationary state is in general not known. The boundaries operators $H_{L / R}$ representing the action of the reservoirs are chosen such that, when the bath parameters are equal $\alpha_{L}=\alpha_{R}=\alpha$ the unique invariant measure is given by the equilibrium Boltzman-Gibbs measure

$$
\begin{equation*}
|\psi\rangle_{\tilde{\alpha}}=\int d x \frac{e^{-\tilde{\alpha} E(x)}}{Z}|x\rangle, \tag{24}
\end{equation*}
$$

where $Z$ is the normalizing partition function
In the following we will denote the equilibrium Boltzman-Gibbs state $|\psi\rangle_{\tilde{\alpha}}$ with $|\tilde{\alpha}\rangle$. In case the system has a discrete configuration space, integrals in all the previous formulas are replaced by discrete sums and Dirac delta functions are replaced by Kronecker delta functions.

The relation between $\alpha$ and $\tilde{\alpha}$ is easy to obtain for each problem using the fact that the equilibrium state $|\tilde{\alpha}\rangle$, see Eq. (24), is annihilated by the boundary 'bath' operators $H_{L / R}(\alpha)$

$$
\begin{equation*}
\left(H_{L / R}(\alpha)\right)|\tilde{\alpha}\rangle=0 \tag{25}
\end{equation*}
$$

This is because, by assumption, the bath terms leave the corresponding equilibrium structure stationary.

## Example A: Hamiltonian systems

A large class of systems is represented by a model composed of $N$ point-like particles interacting with their nearest neighbours. This is described by the Hamiltonian

$$
\begin{equation*}
E=\sum_{i=1}^{N} \frac{p_{i}^{2}}{2}+\sum_{i=1}^{N-1} V\left(q_{i+1}-q_{i}\right) . \tag{26}
\end{equation*}
$$

The evolution equation (11) holds with $x=\left(q_{1}, \ldots, q_{N}, p_{1}, \ldots, p_{N}\right)$ a point in phase space. The bulk evolution operator is the Liouville operator

$$
\begin{equation*}
H_{B}=\{, E\}=\sum_{i=1}^{N} p_{i} \frac{\partial}{\partial q_{i}}-\frac{\partial V}{\partial q_{i}} \frac{\partial}{\partial p_{i}} \tag{27}
\end{equation*}
$$

where $\{$,$\} denotes the Poisson brackets, that is for any functions f$ and $g$

$$
\begin{equation*}
\{f, g\}=\sum_{i=1}^{N} \frac{\partial f}{\partial q_{i}} \frac{\partial g}{\partial p_{i}}-\frac{\partial f}{\partial p_{i}} \frac{\partial g}{\partial q_{i}} \tag{28}
\end{equation*}
$$

The constant of motion for the bulk evolution is the total bulk energy $E$. Indeed $H_{B}$ obviously commutes with the operator that multiplies by $E$ :

$$
\begin{equation*}
H_{B}(E f)=\{E f, E\}=E\{f, E\}+f\{E, E\}=E\{f, E\}=E\left(H_{B} f\right) \quad \forall f \tag{29}
\end{equation*}
$$

To model the interaction with the boundaries, stochastic heat reservoirs can be taken as Ornstein-Uhlenbeck processes whose variances $T_{L / R}$ specify the temperature of the bath. This is represented by boundaries evolution operators

$$
\begin{align*}
-H_{L}\left(T_{L}\right) & =\frac{\partial}{\partial p_{1}}\left(T_{L} \frac{\partial}{\partial p_{1}}+p_{1}\right)  \tag{30}\\
-H_{R}\left(T_{R}\right) & =\frac{\partial}{\partial p_{N}}\left(T_{R} \frac{\partial}{\partial p_{N}}+p_{N}\right) \tag{31}
\end{align*}
$$

When the two thermal reservoirs have the same temperature $T_{L}=T_{R}=T$, the stationary state $|\psi\rangle_{\beta}$ is the Boltzman-Gibbs equilibrium measure

$$
\begin{equation*}
|\psi\rangle_{\beta}=|\beta\rangle=\int d x \frac{e^{-\beta E(x)}}{Z}|x\rangle \tag{32}
\end{equation*}
$$

where the inverse temperature $\beta=1 / T$ is such that

$$
\begin{equation*}
\langle E\rangle=\langle-| E|\beta\rangle=T . \tag{33}
\end{equation*}
$$

Example B: Simple symmetric exclusion process
Another class of models we consider are continuous time Markov processes. With the restriction of a finite configuration space $\mathcal{S}$, the process is specified by assigning the rates of transition $w\left(\sigma^{\prime}, \sigma\right)$ for jumping from a configuration $\sigma \in \mathcal{S}$ to a configuration $\sigma^{\prime} \in \mathcal{S}$. The master equation for $\mu(\sigma, t)$, the probability distribution of a configuration $\sigma$ at time $t$, then reads

$$
\begin{equation*}
\frac{d \mu(\sigma, t)}{d t}=\sum_{\sigma^{\prime} \neq \sigma}\left(w\left(\sigma, \sigma^{\prime}\right) \mu\left(\sigma^{\prime}, t\right)-w\left(\sigma^{\prime}, \sigma\right) \mu(\sigma, t)\right)=-H \mu(\sigma, t) . \tag{34}
\end{equation*}
$$

To be more definite we will work with the simple symmetric exclusion process which can be expressed - in a operator formalism - as an $\mathrm{SU}(2)$ ferromagnet of spin $1 / 2$ [9]. This corresponds to the stochastic process on the lattice $\{1, \ldots, N\}$ where particles jumps at rate 1 to one of their neighbours and each site can accomodate at most 1 particle per site. Configurations $n \in\{0,1\}^{N}$ are then identified with ket states

$$
\begin{equation*}
|n\rangle=\left|n_{1}, \ldots, n_{N}\right\rangle=\otimes_{i=1}^{N}\left|n_{i}\right\rangle, \tag{35}
\end{equation*}
$$

which specify the occupation numbers of each sites, namely $n_{i} \in\{0,1\}$. The bulk evolution is given by the transition rates

$$
\begin{align*}
& w\left(n^{i+1, i}, n\right)=-\left\langle n^{i, i+1}\right| H_{B}|n\rangle=\left(1-n_{i}\right) n_{i+1} \\
& w\left(n^{i, i+1}, n\right)=-\left\langle n^{i, i+1}\right| H_{B}|n\rangle=n_{i}\left(1-n_{i+1}\right) . \tag{36}
\end{align*}
$$

where $n^{i, j}$ is the configuration which is obtained from the configuration $n$ by removing a particle in $i$ and adding it in $j$.

In operator notation, this is generated by [9]

$$
\begin{equation*}
-H_{B}=\sum_{i=1}^{N-1}\left(S_{i}^{+} S_{i+1}^{-}+S_{i}^{-} S_{i+1}^{+}+2 S_{i}^{0} S_{i+1}^{0}-\frac{1}{2}\right) \tag{37}
\end{equation*}
$$

where the $S$ 's operators act as

$$
\begin{align*}
S_{i}^{+}\left|n_{i}\right\rangle & =\left(1-n_{i}\right)\left|n_{i}+1\right\rangle \\
S_{i}^{-}\left|n_{i}\right\rangle & =n_{i}\left|n_{i}-1\right\rangle \\
S_{i}^{0}\left|n_{i}\right\rangle & =\left(n_{i}-\frac{1}{2}\right)\left|n_{i}\right\rangle . \tag{38}
\end{align*}
$$

and satisfy the $\mathrm{SU}(2)$ algebra

$$
\begin{align*}
{\left[S_{i}^{0}, S_{i}^{ \pm}\right] } & = \pm S_{i}^{ \pm} \\
{\left[S_{i}^{-}, S_{i}^{+}\right] } & =-2 S_{i}^{0} \tag{39}
\end{align*}
$$

In this stochastic system the constant of motion - in the absence of reservoirs is the total number of particles

$$
\begin{equation*}
E=\sum_{i=1}^{N}\left(S_{i}^{0}+\frac{1}{2}\right) . \tag{40}
\end{equation*}
$$

This is obviously a conserved quantity for a particle jump process,

$$
\begin{equation*}
\left[E, H_{B}\right]=0, \tag{41}
\end{equation*}
$$

as can be immediately checked using the commutation relations (39).
When the system is coupled to reservoirs at different chemical potential, the boundaries can inject or absorb particle from the system. We assume that particles
are injected at site 1 at rate $\rho_{L}$ and they are removed from site 1 at rate $\left(1-\rho_{L}\right)$; in the same way particles are injected at site $N$ at rate $\rho_{R}$ ) and they are removed from site $N$ at rate $\left(1-\rho_{R}\right)$. The boundaries evolution operators then read

$$
\begin{align*}
& -H_{L}\left(\rho_{L}\right)=\rho_{L}\left(S_{1}^{+}+S_{1}^{0}-\frac{1}{2}\right)+\left(1-\rho_{L}\right)\left(S_{1}^{-}-S_{1}^{0}-\frac{1}{2}\right)  \tag{42}\\
& -H_{R}\left(\rho_{R}\right)=\rho_{R}\left(S_{N}^{+}+S_{N}^{0}-\frac{1}{2}\right)+\left(1-\rho_{R}\right)\left(S_{N}^{-}-S_{N}^{0}-\frac{1}{2}\right) \tag{43}
\end{align*}
$$

The constants $\rho_{L}$ and $\rho_{R}$ are to interpreted as the two densities the reservoirs would impose if acting separately. When the two reservoirs have the same densities $\rho_{L}=$ $\rho_{R}=\rho$, the stationary state $|\psi\rangle_{\nu}$ is the Boltzman-Gibbs equilibrium measure

$$
\begin{equation*}
|\psi\rangle_{\nu}=|\nu\rangle=\sum_{\{n\}} \frac{e^{\nu E}}{Z}|n\rangle, \tag{44}
\end{equation*}
$$

where the chemical potential $\nu=\ln \left(\frac{\rho}{1-\rho}\right)$ is such that

$$
\begin{equation*}
\langle E\rangle=\langle-| E|\nu\rangle=\rho . \tag{45}
\end{equation*}
$$

As it is immediately checked, in this case the equilibrium Gibbs measure is a Bernoulli product measure with parameter $\rho=e^{\nu} /\left(1+e^{\nu}\right)$

$$
\begin{equation*}
|\rho\rangle=\otimes_{i=1}^{N}|\rho\rangle_{i}=\otimes_{i=1}^{N}\left(\rho|1\rangle_{i}+(1-\rho)|0\rangle_{i}\right) . \tag{46}
\end{equation*}
$$

## 4 Bulk current and 'helical' operator

We wish to study the transport of the quantity $E$ in the presence of reservoirs. Our first step is to express the current in the bulk in terms of a 'helical' operator.

The current which passes through the system is defined via the continuity equation

$$
\begin{equation*}
\frac{d E}{d t}+\nabla \mathcal{J}=0 \tag{47}
\end{equation*}
$$

Since $E$ is the sum of $N$ local contributions, see Eq.(3), we can write a local continuity equation as

$$
\begin{equation*}
\frac{d E_{s}}{d t}=-\left(\mathcal{J}_{s, s+1}-\mathcal{J}_{s-1, s}\right), \quad \quad s=1, \ldots, N \tag{48}
\end{equation*}
$$

where $\mathcal{J}_{s, s+1}$ is the current from site $s$ to site $s+1$, and the total bulk current is defined as

$$
\begin{equation*}
\mathcal{J}=\sum_{s=1}^{N-1} \mathcal{J}_{s, s+1} \tag{49}
\end{equation*}
$$

For a stochastic system, $\mathcal{J}_{s, s+1}$ may depend explicitely on the random noise. We shall consider a set of operators $J_{s, s+1}$ such that they coincide with the average of $\mathcal{J}_{s, s+1}$ over random realisations

$$
\begin{equation*}
\left\langle\mathcal{J}_{s, s+1}(t)\right\rangle_{\text {noise }}=\langle-| J_{s, s+1}|\Psi(t)\rangle \quad ; \quad\langle\mathcal{J}(t)\rangle_{\text {noise }}=\langle-| J|\Psi(t)\rangle \tag{50}
\end{equation*}
$$

Defining the helical operator

$$
\begin{equation*}
A=\sum_{s=1}^{N} s E_{s} \tag{51}
\end{equation*}
$$

$J$ can be expressed as the commutator between it and the bulk evolution operator, that is

$$
\begin{equation*}
J=\left[A, H_{B}\right] \tag{52}
\end{equation*}
$$

Indeed, for an open chain (namely $\lambda=0$ ) we have

$$
\begin{equation*}
\langle-|\left[\left[A, H_{B}\right]-\frac{d A}{d t}\right]|\Psi(t)\rangle=0 \tag{53}
\end{equation*}
$$

Making use of the continuity equation (48), we then have

$$
\begin{equation*}
\langle-|\left[A, H_{B}\right]|\Psi(t)\rangle=\langle-| \frac{d A}{d t}|\Psi(t)\rangle=\sum_{s=1}^{N} s\langle-| \frac{d E_{s}}{d t}|\Psi(t)\rangle=\sum_{s=1}^{N} s\left\langle\mathcal{J}_{s-1, s}-\mathcal{J}_{s, s+1}\right\rangle \tag{54}
\end{equation*}
$$

Since $\mathcal{J}_{0,1}=\mathcal{J}_{N, N+1}=0$ for an open chain:

$$
\begin{equation*}
\langle-|\left[A, H_{B}\right]|\Psi(t)\rangle=\sum_{s=2}^{N} s\langle-| J_{s-1, s}|\Psi(t)\rangle-\sum_{s=1}^{N-1} s\langle-| J_{s, s+1}|\Psi(t)\rangle \tag{55}
\end{equation*}
$$

and making the change $s \rightarrow s+1$ in the first summation we find

$$
\begin{equation*}
\langle-|\left[A, H_{B}\right]|\Psi(t)\rangle=\sum_{s=1}^{N-1}\left\langle\mathcal{J}_{s, s+1}\right\rangle=\langle\mathcal{J}\rangle=\langle-| J|\Psi(t)\rangle \tag{56}
\end{equation*}
$$

Remark 1: The correspondence between $J$ and $\mathcal{J}$ is via expectation values. Note however that expectations of products yield extra terms in stochastic systems: $\left\langle\mathcal{J}^{2}\right\rangle=\langle-| J^{2}|\Psi\rangle+$ extra trems. This is the origin of extra terms in the formulas below.

Remark: 2 In the definition of the helical operator one can always add a term whose total derivative with respect to time is zero. Later, to make the role of the boundaries more symmetric, we will consider

$$
\begin{equation*}
A=\sum_{s=1}^{N} s E_{s}-\frac{N+1}{2} E \tag{57}
\end{equation*}
$$

Example A: Hamiltonian system
For the system described by the Hamiltonian (26) the current from site $s$ to site $s+1$ is given by (see [2])

$$
\begin{equation*}
\mathcal{J}_{s, s+1}=-\frac{1}{2}\left(p_{s}+p_{s+1}\right) V^{\prime}\left(q_{s+1}-q_{s}\right) \tag{58}
\end{equation*}
$$

Defining the local operators $E_{s}$ as

$$
\begin{align*}
E_{1} & =\frac{p_{1}^{2}}{2}+\frac{1}{2} V\left(q_{2}-q_{1}\right) \\
E_{s} & =\frac{p_{s}^{2}}{2}+\frac{1}{2}\left(V\left(q_{s+1}-q_{s}\right)+V\left(q_{s}-q_{s-1}\right)\right) \quad s=2, \ldots, N-1 \\
E_{N} & =\frac{p_{N}^{2}}{2}+\frac{1}{2} V\left(q_{N}-q_{N-1}\right) \tag{59}
\end{align*}
$$

one can check that (52) holds with

$$
\begin{align*}
A & =\sum_{s=1}^{N} s E_{s}-\frac{N+1}{2} E \\
& =\sum_{s=1}^{N} s \frac{p_{s}^{2}}{2}+\sum_{s=1}^{N-1}(2 s+1) V\left(q_{s+1}-q_{s}\right)-\frac{N+1}{2} E \tag{60}
\end{align*}
$$

## Example B: Simple symmetric exclusion process

For the system described by the evolution operator (37) the current from site $s$ to site $s+1$ is

$$
\begin{equation*}
J_{s, s+1}=S_{s}^{-} S_{s+1}^{+}-S_{s}^{+} S_{s+1}^{-} \tag{61}
\end{equation*}
$$

Equation (52) now holds with

$$
\begin{align*}
A & =\sum_{s=1}^{N} s E_{s}-\frac{N+1}{2} E \\
& =\sum_{s=1}^{L} s\left(S_{s}^{0}+\frac{1}{2}\right)-\frac{N+1}{2} E \tag{62}
\end{align*}
$$

### 4.1 A useful general identity

The boundary terms $H_{L / R}(\alpha)$ break the conservation law for the quantity $E$. They depend on a parameter $\alpha$ (e.g. the temperature in the Hamiltonian system example, the chemical potential in the symmetric exclusion process example) and impose a unique stationary equilibrium Boltzmann Gibbs state $|\psi\rangle_{\tilde{\alpha}}=|\tilde{\alpha}\rangle$. We wish to find a convenient way to express the response of the boundary operators $H_{L / R}(\alpha)$ when their parameter $\alpha$ is varied. We claim the following identities hold:

$$
\begin{equation*}
\left(\frac{\partial}{\partial \alpha} H_{L / R}(\alpha)\right)|\tilde{\alpha}\rangle=c_{\alpha}\left[H_{L / R}(\alpha), E\right]|\tilde{\alpha}\rangle \tag{63}
\end{equation*}
$$

where the constant $c_{\alpha}$ is given by

$$
\begin{equation*}
c_{\alpha}=\frac{\partial \tilde{\alpha}}{\partial \alpha} . \tag{64}
\end{equation*}
$$

This can be proved as follows. We use the fact that the Gibbs-Boltzmann distribution is annihilated by the boundary operators (cfr Eq. (25)), and that, because of the Gibbs-Boltzmann form, it satisfies:

$$
\begin{equation*}
\frac{\partial}{\partial \tilde{\alpha}}|\tilde{\alpha}\rangle=-(E-\langle E\rangle)|\tilde{\alpha}\rangle \tag{65}
\end{equation*}
$$

where $\langle E\rangle=\langle-| E|\tilde{\alpha}\rangle$. Computing the derivative of Eq.(25) with respect to $\tilde{\alpha}$, this in turn gives:

$$
\begin{align*}
0 & =\left(\frac{\partial}{\partial \tilde{\alpha}} H_{L / R}(\alpha)\right)|\tilde{\alpha}\rangle+H_{L / R}(\alpha) \frac{\partial}{\partial \tilde{\alpha}}|\tilde{\alpha}\rangle \\
& =\left(\frac{\partial}{\partial \tilde{\alpha}} H_{L / R}(\alpha)\right)|\tilde{\alpha}\rangle-H_{L / R}(\alpha)(E-\langle E\rangle)|\tilde{\alpha}\rangle \\
& =\left(\frac{\partial}{\partial \tilde{\alpha}} H_{L / R}(\alpha)\right)|\tilde{\alpha}\rangle-\left[H_{L / R}(\alpha), E\right]|\tilde{\alpha}\rangle \tag{66}
\end{align*}
$$

where we have used (65). Eq. (63) then follows.
Example A: Hamiltonian system
Eq. (63) holds with $\alpha=T, \tilde{\alpha}=\beta=\frac{1}{T}$ and with $c_{T}=-\frac{1}{T^{2}}$.
Example B: Simple symmetric exclusion process
Eq. (63) holds with $\alpha=\rho, \tilde{\alpha}=-\nu=\ln \left(\frac{1-\rho}{\rho}\right)$ and with $c_{\rho}=-\frac{1}{\rho(1-\rho)}$.

## 5 Linear response theory

The conductivity is obtained by calculating the average current in the presence of a small mismatch in the parameters of the reservoirs evolution operators. If the left reservoir is working with a parameter $\alpha_{L}=\alpha-\delta \alpha$ and the right reservoir is working with a parameter $\alpha_{R}=\alpha+\delta \alpha$, the evolution equation

$$
\begin{equation*}
\frac{d}{d t}|\psi(t)\rangle=-H|\psi(t)\rangle \tag{67}
\end{equation*}
$$

can be solved in a linear response regime. Expanding to first order in $\delta \alpha$ we find

$$
\begin{equation*}
H=H_{0}+\delta \alpha \lambda \Delta H+o(\delta \alpha) \tag{68}
\end{equation*}
$$

with

$$
\begin{equation*}
H_{0}=H_{B}+\lambda\left(H_{R}(\alpha)+H_{L}(\alpha)\right) \tag{69}
\end{equation*}
$$

$$
\begin{equation*}
\Delta H=\left(\frac{\partial}{\partial \alpha} H_{R}-\frac{\partial}{\partial \alpha} H_{L}\right) \tag{70}
\end{equation*}
$$

and

$$
\begin{equation*}
|\psi(t)\rangle=|\tilde{\alpha}\rangle+\delta \alpha|\Delta \psi(t)\rangle+o(\delta \alpha) \tag{71}
\end{equation*}
$$

with $|\tilde{\alpha}\rangle$ is the stationary state for the unperturbed problem, that is

$$
\begin{equation*}
\frac{d}{d t}|\tilde{\alpha}\rangle=-H_{0}|\tilde{\alpha}\rangle=0 \tag{72}
\end{equation*}
$$

The solution is

$$
\begin{equation*}
|\Delta \psi(t)\rangle=-\lambda \int_{0}^{t} d t^{\prime} e^{-\left(t-t^{\prime}\right) H} \Delta H|\tilde{\alpha}\rangle \tag{73}
\end{equation*}
$$

To leading order the average value of the total bulk current will be

$$
\begin{align*}
\langle\mathcal{J}(t)\rangle & =\langle-| J|\psi(t)\rangle \\
& =\langle-| J|\tilde{\alpha}\rangle-\delta \alpha \lambda \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} \Delta H|\tilde{\alpha}\rangle+o(\delta \alpha) \tag{74}
\end{align*}
$$

The conductivity $\kappa_{N}$ for a system of size $N$ is defined as

$$
\begin{equation*}
\kappa_{N}=\lim _{t \rightarrow \infty} \frac{\delta\langle\mathcal{J}(t)\rangle}{2 \delta \alpha} \tag{75}
\end{equation*}
$$

From Eq.(74) the following formula for the conductivity is then deduced:

$$
\begin{equation*}
\kappa_{N}=\lim _{t \rightarrow \infty}-\frac{\lambda}{2} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} \Delta H|\tilde{\alpha}\rangle \tag{76}
\end{equation*}
$$

Thanks to the previous established (63), we have:

$$
\begin{equation*}
\Delta H|\tilde{\alpha}\rangle=-c_{\alpha} H^{\prime}|\tilde{\alpha}\rangle \tag{77}
\end{equation*}
$$

where we have defined

$$
\begin{equation*}
H^{\prime}=\left[H_{L}-H_{R}, E\right] . \tag{78}
\end{equation*}
$$

Substituting in (76), we then have

$$
\begin{equation*}
\kappa_{N}=\lim _{t \rightarrow \infty} \frac{\lambda c_{\alpha}}{2} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \tag{79}
\end{equation*}
$$

### 5.1 Green-Kubo formula in the bulk

The Green-Kubo formula for the conductivity usually involves the current temporal autocorrelation function [10]. To see that formula (79) is indeed the standard Green-Kubo formula we proceed further by using some properties of the reservoirs. Specifically, we use the assumption that the reservoir on the left (resp. on the right)
depends only from the phase/configuration variables of the first (resp. last) site. This implies that

$$
\begin{align*}
\frac{1}{N}\left[A, H_{L}+H_{R}\right] & =\frac{1}{N}\left[\sum_{s=1}^{N} s E_{s}-\frac{N+1}{2} \sum_{s=1}^{N} E_{s}, H_{L}+H_{R}\right] \\
& =\frac{1}{N}\left[\left(\frac{1-N}{2}\right) E_{1}, H_{L}\right]+\frac{1}{N}\left[\frac{N-1}{2} E_{N}, H_{R}\right] \\
& =\frac{N-1}{2 N}\left[H_{L}-H_{R}, E\right] \\
& =\frac{N-1}{2 N} H^{\prime} \tag{80}
\end{align*}
$$

On the other hand, we also have

$$
\begin{equation*}
\frac{1}{N}\left[A, H_{R}+H_{L}\right]=\frac{1}{\lambda N}\left[A, H-H_{B}\right]=-\frac{1}{\lambda N}[H, A]-\frac{J}{\lambda N} \tag{81}
\end{equation*}
$$

Putting (80) and (81) together we find

$$
\begin{equation*}
\frac{1}{2} H^{\prime}=-\frac{1}{\lambda(N-1)}(J+[H, A]) \tag{82}
\end{equation*}
$$

The standard Green-Kubo formula is obtained by substituting $H^{\prime}$ on the right of (79) by the expression found in Eq. (82). We have

$$
\begin{align*}
\kappa_{N}= & -\lim _{t \rightarrow \infty} \frac{c_{\alpha}}{N-1} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\tilde{\alpha}\rangle \\
& -\lim _{t \rightarrow \infty} \frac{c_{\alpha}}{N-1} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H}[H, A]|\tilde{\alpha}\rangle \tag{83}
\end{align*}
$$

The term involving the commutator $[H, A]$ can be further simplified as follows

$$
\begin{align*}
\lim _{t \rightarrow \infty} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} H A|\tilde{\alpha}\rangle & =\lim _{t \rightarrow \infty} \int_{0}^{t} d t^{\prime} \frac{d}{d t^{\prime}}\langle-| J e^{-\left(t-t^{\prime}\right) H} A|\tilde{\alpha}\rangle \\
& =\langle-| J A|\tilde{\alpha}\rangle \tag{84}
\end{align*}
$$

where we have used that $H|\tilde{\alpha}\rangle=0$ and we have assumed that the $J$ and $A$ have vanishing correlation for very large times. Moreover, by using (52) and the fact that $H_{B}|\tilde{\alpha}\rangle=\langle-| H_{B}=0$, one has that

$$
\begin{align*}
\langle-| J A|\tilde{\alpha}\rangle & =\langle-|\left[A, H_{B}\right] A|\tilde{\alpha}\rangle \\
& =\langle-| A H_{B} A|\tilde{\alpha}\rangle \\
& =\frac{1}{2}\langle-|\left[\left[A, H_{B}\right], A\right]|\tilde{\alpha}\rangle \tag{85}
\end{align*}
$$

Finally we get

$$
\begin{equation*}
\kappa_{N}=-\lim _{t \rightarrow \infty} \frac{c_{\alpha}}{N-1} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\tilde{\alpha}\rangle-\frac{c_{\alpha}}{2(N-1)}\langle-|\left[\left[A, H_{B}\right], A\right]|\tilde{\alpha}\rangle \tag{86}
\end{equation*}
$$

The second term comes from the fact, already mentioned above, that $\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\tilde{\alpha}\rangle$ is, in stochastic systems, the current-current correlation function only up to an equaltime extra term. We distinguish two cases:

- $\lambda=0$

In this case $H_{\lambda}=H_{B}$ and then the current autocorrelation function can be treated as we just did for the extra term:

$$
\begin{align*}
\lim _{t \rightarrow \infty} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H_{B}} J|\tilde{\alpha}\rangle & =\lim _{t \rightarrow \infty} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H_{B}} H_{B} A|\tilde{\alpha}\rangle \\
& =\lim _{t \rightarrow \infty} \int_{0}^{t} d t^{\prime} \frac{d}{d t^{\prime}}\langle-| J e^{-\left(t-t^{\prime}\right) H_{B}} A|\tilde{\alpha}\rangle \\
& =\langle-| J A|\tilde{\alpha}\rangle \\
& =\frac{1}{2}\langle-|\left[\left[A, H_{B}\right], A\right]|\tilde{\alpha}\rangle . \tag{87}
\end{align*}
$$

This implies that the two terms in Eq. (86) cancel each others and, consistently with the fact that there is no coupling to the reservoirs, we find $\kappa_{N}=0$ (see Ref. [6] for a discussion)

- $\lambda \neq 0$

This time $\kappa_{N}$ is different from zero and is, in general, the sum of two competing terms: the time integral of the current autocorrelation function and an extraterm which is purely due to randomness.

## Example A: Hamiltonian system

The commutator in Eq. (86) vanishes in the Hamiltonian case. Indeed we have:

$$
\begin{equation*}
\left[A, H_{B}\right] f=A\{E, f\}-\{E, A f\} \quad \forall f \tag{88}
\end{equation*}
$$

from which it follows that

$$
\begin{align*}
{\left[\left[A, H_{B}\right], A\right] f } & =\left[A, H_{B}\right] A f-A\left[A, H_{B}\right] f \\
& =A\{E, A f\}-\left\{E, A^{2} f\right\}-A^{2}\{E, f\}+A\{E, A f\} \\
& =0 \tag{89}
\end{align*}
$$

Inserting $\alpha=T$ and $c_{T}=-\frac{1}{T^{2}}$ into (86), the Green-Kubo formula for the conductivity then reads

$$
\begin{equation*}
\kappa_{N}=\lim _{t \rightarrow \infty} \frac{1}{T^{2}(N-1)} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\beta\rangle \tag{90}
\end{equation*}
$$

Example B: Simple symmetric exclusion process

In this case the commutator in Eq. (86) is non-zero. We have

$$
\begin{equation*}
\left[A, H_{B}\right]=J=\sum_{s=1}^{N-1}\left(S_{s}^{-} S_{s+1}^{+}-S_{s}^{+} S_{s+1}^{-}\right) \tag{91}
\end{equation*}
$$

and

$$
\begin{equation*}
\left[\left[A, H_{B}\right], A\right]=-\sum_{s=1}^{N-1}\left(S_{s}^{-} S_{s+1}^{+}+S_{s}^{+} S_{s+1}^{-}\right) \tag{92}
\end{equation*}
$$

Recalling that for the SSEP with reservoirs having the same chemical potential the equilibrium state is given by a Bernoulli product measure, see Eq. (46), an immediate computation gives

$$
\begin{equation*}
\langle-|\left[\left[A, H_{B}\right], A\right]|\tilde{\alpha}\rangle=-2 \rho(1-\rho)(N-1) \tag{93}
\end{equation*}
$$

This implies the following expression for the conductivity:

$$
\begin{equation*}
\kappa_{N}=-1+\lim _{t \rightarrow \infty} \frac{1}{(N-1) \rho(1-\rho)} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\rho\rangle \tag{94}
\end{equation*}
$$

As a final remark of this section, let us check that in the thermodynamical limit the correct value of the conductivity is recovered. In order to evaluate the contribution due to the current autocorrelation function we observe that in the thermodynamic limit $N \rightarrow \infty$, whatever the value of $\lambda<\infty$, the boundaries will be negligible. This lead us to evaluate this term for the infinite volume system:

$$
\begin{align*}
& \lim _{N \rightarrow \infty} \lim _{t \rightarrow \infty} \frac{1}{(N-1) \rho(1-\rho)} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\rho\rangle= \\
& =\frac{2}{\rho(1-\rho)} \int_{0}^{\infty} d t^{\prime}<\mathcal{J}_{0,1}(0) \mathcal{J}_{0,1}\left(t^{\prime}\right)> \tag{95}
\end{align*}
$$

where $<\cdot>$ denotes expectation with respect to the equilibrium state. We can then use the duality property for the model and specifically the following results:

$$
\begin{equation*}
<\left(n_{x}(t)-\rho\right)\left(n_{0}(0)-\rho\right)>=\rho(1-\rho) p_{t}(x) \tag{96}
\end{equation*}
$$

where $p_{t}(x)$ is the probability that a continuous time simple symmetric random walk jumping left or right at rate 1 , started at the origin at time zero, is found at site $x$ at time $t$. Using duality we have

$$
\begin{align*}
<\mathcal{J}_{0,1}(0) \mathcal{J}_{0,1}\left(t^{\prime}\right)> & =<\left(n_{1}(0)-n_{0}(0)\right)\left(n_{1}\left(t^{\prime}\right)-n_{0}\left(t^{\prime}\right)\right)> \\
& =\rho(1-\rho)\left(-p_{t^{\prime}}(-1)+2 p_{t^{\prime}}(0)-p_{t}(1)\right) \\
& =-\rho(1-\rho) \frac{d}{d t^{\prime}} p_{t^{\prime}}(0) \tag{97}
\end{align*}
$$

Putting together (95) and (97) we arrive to

$$
\begin{align*}
\lim _{N \rightarrow \infty} \lim _{t \rightarrow \infty} \frac{1}{(N-1) \rho(1-\rho)} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} J|\rho\rangle & =-2\left(p_{\infty}(0)-p_{0}(0)\right) \\
& =2 \tag{98}
\end{align*}
$$

Inserting this result in Eq. (94) we finally find (as it should be!):

$$
\begin{equation*}
k=\lim _{N \rightarrow \infty} \kappa_{N}=-1+2=1 \tag{99}
\end{equation*}
$$

### 5.2 Green-Kubo formula for the boundaries

Here we follow the opposite strategy of the previous section. Recall expression (79) for the conductivity:

$$
\begin{equation*}
\kappa_{N}=\lim _{t \rightarrow \infty} \frac{\lambda c_{\alpha}}{2} \int_{0}^{t} d t^{\prime}\langle-| J e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \tag{100}
\end{equation*}
$$

This time we express $J$ in terms of $H^{\prime}$ by inverting relation (82), that is:

$$
\begin{equation*}
J=-\frac{\lambda(N-1)}{2} H^{\prime}-[H, A] \tag{101}
\end{equation*}
$$

This yields the following expression

$$
\begin{align*}
\kappa_{N}= & -\lim _{t \rightarrow \infty} \frac{\lambda^{2} c_{\alpha}(N-1)}{4} \int_{0}^{t} d t^{\prime}\langle-| H^{\prime} e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \\
& -\lim _{t \rightarrow \infty} \frac{\lambda c_{\alpha}}{2} \int_{0}^{t} d t^{\prime}\langle-|[H, A] e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \tag{102}
\end{align*}
$$

As in the previous case the term involving the commutator $[H, A]$ can be simplified by using the fact that it is the integral of a time-derivative, and that the correlations of $A$ and $H^{\prime}$ vanish at widely separated times:

$$
\begin{align*}
\kappa_{N}= & -\lim _{t \rightarrow \infty} \frac{\lambda^{2} c_{\alpha}(N-1)}{4} \int_{0}^{t} d t^{\prime}\langle-| H^{\prime} e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \\
& -\frac{\lambda c_{\alpha}}{2}\langle-| A H^{\prime}|\tilde{\alpha}\rangle \tag{103}
\end{align*}
$$

The extra term can be rearranged as follows. Recalling the definition of $H^{\prime}$, Eq. (78), and using the fact that $H_{L}$ and $H_{R}$ annihilate the equilibrium measure we have

$$
\begin{align*}
\langle-| A H^{\prime}|\tilde{\alpha}\rangle & =\langle-| A\left[H_{L}-H_{R}, E\right]|\tilde{\alpha}\rangle \\
& =\langle-| A\left(H_{L}-H_{R}\right) E|\tilde{\alpha}\rangle \tag{104}
\end{align*}
$$

Now we use that $H_{L}\left(\right.$ resp. $\left.H_{R}\right)$ commutes with all the $E_{i}$ with $i \neq 1($ resp. $i \neq N)$. This yields:

$$
\begin{align*}
\langle-| A H^{\prime}|\tilde{\alpha}\rangle & \left.=-\frac{N-1}{2}\langle-| E\left(H_{L}+H_{R}\right) E\right]|\tilde{\alpha}\rangle \\
& =\frac{N-1}{4}\langle-|\left[E,\left[E, H_{L}+H_{R}\right]\right]|\tilde{\alpha}\rangle \tag{105}
\end{align*}
$$

and the final expression for the Green-Kubo formula for the boundaries read:

$$
\begin{align*}
\kappa_{N}= & -\lim _{t \rightarrow \infty} \frac{\lambda^{2} c_{\alpha}(N-1)}{4} \int_{0}^{t} d t^{\prime}\langle-| H^{\prime} e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \\
& -\frac{\lambda c_{\alpha}(N-1)}{8}\langle-|\left[E,\left[E, H_{L}+H_{R}\right]\right]|\tilde{\alpha}\rangle \tag{106}
\end{align*}
$$

We will show below that the extra term is non-zero for both the Hamiltonian chain and the SEP and has actually the same value.

Example A: Hamiltonian system
The extra term is evaluated as

$$
\begin{align*}
\langle-|\left[E,\left[E, H_{L}+H_{R}\right]\right]|\beta\rangle & =\langle-|\left[E_{1},\left[E_{1}, H_{L}\right]\right]|\beta\rangle+\langle-|\left[E_{N},\left[E_{N}, H_{R}\right]\right]|\beta\rangle \\
& =-2\langle-| E_{1} H_{L} E_{1}|\beta\rangle-2\langle-|\left[E_{N} H_{R} E_{N}|\beta\rangle\right. \tag{107}
\end{align*}
$$

We have

$$
\begin{align*}
\langle-| E_{1} H_{L} E_{1}|\beta\rangle & =-\langle-| \frac{p_{1}^{2}}{2} \frac{\partial}{\partial p_{1}}\left(T \frac{\partial}{\partial p_{1}}+p_{1}\right) \frac{p_{1}^{2}}{2}|\beta\rangle \\
& =T\langle-| p_{1}^{2}|\beta\rangle \\
& =T^{2} \tag{108}
\end{align*}
$$

where we have used the fact that $\frac{\partial}{\partial p_{1}}$ annihilates the flat measure to the left and $\left(T \frac{\partial}{\partial p_{1}}+p_{1}\right)$ annihilates the equilibrium measure to the right, together with

$$
\begin{gather*}
{\left[\frac{p_{1}^{2}}{2}, \frac{\partial}{\partial p_{1}}\right]=-p_{1}}  \tag{109}\\
{\left[T \frac{\partial}{\partial p_{1}}+p_{1}, \frac{p_{1}^{2}}{2}\right]=T p_{1}} \tag{110}
\end{gather*}
$$

Analogously we find that

$$
\begin{equation*}
\langle-| E_{N} H_{R} E_{N}|\beta\rangle=T^{2} \tag{111}
\end{equation*}
$$

so that the final result for the extra term in the thermodynamic limit is:

$$
\begin{equation*}
\frac{\lambda c_{\alpha}(N-1)}{8}\langle-|\left[E,\left[E, H_{L}+H_{R}\right]\right]|\beta\rangle=\frac{\lambda(N-1)}{2} \tag{112}
\end{equation*}
$$

Example B: Simple symmetric exclusion process
With

$$
\begin{equation*}
H_{L}=-\rho\left(S_{1}^{+}+S_{1}^{0}-\frac{1}{2}\right)-(1-\rho)\left(S_{1}^{-}-S_{1}^{0}-\frac{1}{2}\right) \tag{113}
\end{equation*}
$$

we have

$$
\begin{align*}
\langle-|\left[E,\left[E, H_{L}\right]\right]|\rho\rangle & =\langle-|\left[E_{1},\left[E_{1}, H_{L}\right]\right]|\rho\rangle \\
& =\langle-|-\rho S_{1}^{+}-(1-\rho) S_{1}^{-}|\rho\rangle \tag{114}
\end{align*}
$$

Because $\left(S_{1}^{+}+S_{1}^{0}-\frac{1}{2}\right)$ and ( $S_{1}^{-}-S_{1}^{0}-\frac{1}{2}$ ) separately annihilate the flat measure, we can substitute $S_{1}^{ \pm}$by $S_{1}^{0}$ 's to get

$$
\begin{align*}
\langle-|\left[E,\left[E, H_{L}\right]\right]|\rho\rangle & =\langle-| \rho\left(S_{1}^{0}-\frac{1}{2}\right)+(1-\rho)\left(-S_{1}^{0}-\frac{1}{2}\right)|\rho\rangle \\
& =-\rho(1-\rho)-(1-\rho) \rho \\
& =-2 \rho(1-\rho) \tag{115}
\end{align*}
$$

The extra term is then:

$$
\begin{equation*}
\frac{\lambda c_{\alpha}(N-1)}{8}\langle-|\left[E,\left[E, H_{L}+H_{R}\right]\right]|\rho\rangle=\frac{\lambda(N-1)}{2} \tag{116}
\end{equation*}
$$

## 6 Stiffness

Let us now compute the stiffness. We have a 'quantum-like' Hamiltonian $H=$ $H_{B}+\lambda\left(H_{L}+H_{R}\right)$ where the bulk term is "symmetric" with respect to transformations generated by $E$, since $\left[H_{B}, E\right]=0 . H_{L}$ and $H_{R}$ are the boundary 'handles' that break the symmetry generated by $E$. In order to calculate the stiffness, we twist the boundaries, i.e. we apply the transformation in opposite directions:

$$
\begin{equation*}
H_{L} \rightarrow H_{L}^{\theta}=e^{i \theta E} H_{L} e^{-i \theta E} \quad H_{R} \rightarrow H_{R}^{\theta}=e^{-i \theta E} H_{R} e^{i \theta E} \tag{117}
\end{equation*}
$$

As a consequence of the twist the spectrum of the transformed Hamiltonian $H^{\theta}=$ $H_{B}+\lambda\left(H_{L}^{\theta}+H_{R}^{\theta}\right)$ will be different from the one of the original Hamiltonian $H$. We define the stiffness $\sigma$ in terms of the lowest eigenvalue of $H^{\theta}$ :

$$
\begin{equation*}
\epsilon^{\theta}=-\lim _{t \rightarrow \infty} \frac{\ln \left(\langle-| e^{-t H^{\theta}}|\psi(t)\rangle\right)}{t} \tag{118}
\end{equation*}
$$

We define

$$
\begin{equation*}
H^{\theta}=H_{L}^{\theta}+H_{R}^{\theta} \tag{119}
\end{equation*}
$$

Developing up to order $\theta^{2}$ we have

$$
\begin{aligned}
\Delta H & \equiv H^{\theta}-H=e^{i \theta E} H_{L} e^{-i \theta E}+e^{-i \theta E} H_{R} e^{i \theta E}-\left(H_{L}-H_{R}\right) \\
& =-i \theta H^{\prime}-\frac{\theta^{2}}{2}\left(\left[E,\left[E, H_{L}+H_{R}\right]\right]\right)+\ldots
\end{aligned}
$$

Application of time-dependent perturbation theory gives

$$
\left.\begin{array}{rl}
\ln \left(\langle-| e^{-t \tilde{H}}|\psi(t)\rangle\right)= & \ln (1 \tag{120}
\end{array}+\lambda \int_{0}^{t} d t^{\prime}\langle-| \Delta \tilde{H}|\tilde{\alpha}\rangle\right)
$$

We find for the increase in the lowest eigenvalue

$$
\begin{aligned}
\epsilon^{\theta}-\epsilon^{o} \sim & \frac{1}{2} \frac{\sigma_{N}}{(N-1)}(2 \theta)^{2} \\
= & -\lim _{t \rightarrow \infty} \frac{\ln \left(\langle-| e^{-t \tilde{H}}|\psi(t)\rangle\right)}{t} \\
= & -\lim _{t \rightarrow \infty} \frac{\theta^{2} \lambda}{2}\langle-|\left(\left[E,\left[E, H_{L}+H_{R}\right]\right]\right)|\tilde{\alpha}\rangle \\
& -\lim _{t \rightarrow \infty} \theta^{2} \lambda^{2} \int_{0}^{t} d t^{\prime}\langle-| H^{\prime} e^{-\left(t-t^{\prime}\right) H_{B}} H^{\prime}|\tilde{\alpha}\rangle
\end{aligned}
$$

Recalling the expression (106) for the conductivity

$$
\begin{align*}
\frac{2 \kappa_{N}}{c_{\alpha}(N-1)}= & -\lim _{t \rightarrow \infty} \frac{\theta^{2} \lambda^{2}}{2} \int_{0}^{t} d t^{\prime}\langle-| H^{\prime} e^{-\left(t-t^{\prime}\right) H} H^{\prime}|\tilde{\alpha}\rangle \\
& -\lim _{t \rightarrow \infty} \frac{\theta^{2} \lambda}{4}\langle-|\left[E,\left[E, H_{L}+H_{R}\right]\right]|\tilde{\alpha}\rangle \tag{121}
\end{align*}
$$

one obtains the following relation between the conductivity and the stiffness:

$$
\begin{equation*}
\kappa_{N}=c_{\alpha} \sigma_{N} . \tag{122}
\end{equation*}
$$

Stiffness and conductivity are proportional up to a trivial factor.

## 7 Conclusions

When a system has a conserved bulk quantity, its bulk evolution operator has a symmetry. Current transport induced by boundary 'reservoir' terms corresponds in all generality to a twist exerted applying the symmetry transformation in opposite senses to the boundary terms. The conductivity of the system is in this view the stiffness, or helicity modulus, associated with this operation.

This mechanical analogy of transport can be taken further. For example, one easily understands that in an elastic system any local perturbation that couples with
torsion will have long-range effects: the analogy discussed here means that the same can be said of perturbations of systems with conserved quantities [11.

In fact, one recognizes methods where auxiliary thermal baths are used, with their temperature fixed so that they exchange no current on average [12] as the usual symmetry-breaking fields, adjusted so that they exert no average force, of statistical mechanics.

The derivation in this paper was made for classical and stochastic systems, in contact with reservoirs at the ends. The generalization to a quantum system with baths can be made through the Feyman-Vernon [13] formalism. It is not at this point clear to us how this may be related to the approach of Kohn [4] and Shastry and Sutherland [5], where the twist is applied to the Hamiltonian (rather than the evolution operator) of a closed chain.

## References

[1] F. Bonetto, J. Lebowitz, L. Rey-Bellet, "Fourier's Law: a Challenge for Theorists", in Mathematical Physics 2000, A. Fokas, A. Grigoryan, T. Kibble and B. Zegarlinsky (Eds.), Imperial College, London, (2000), pp. 128-150.
[2] S. Lepri, R. Livi, A. Politi, Phys. Rep. 3771 (2003).
[3] Z. Rieder, J.L. Lebowitz, E. Lieb, J. Math. Phys. 81073 (1967).
[4] W. Kohn, Phys. Rev. 133, A171 (1964).
[5] B.S. Shastry, B. Sutherland, Phys. Rev. Lett. 65, 243 (1990).
[6] M. Rigol, B. S. Shastry, Phys. Rev. B 77, 161101(R) (2008).
[7] M.E. Fisher and M.N. Barber, Phys. Rev. A 8, 1111 (1973).
[8] In this sense, it is close in spirit to the treatment in: P. Gaspard, Phys. Rev. E 53, 4379 (1996).
[9] G. Schtz and S. Sandow, Phys. Rev. E 49, 2726 (1994).
[10] R. Kubo, M. Toda, N. Hashitsume, Statistical Physics II: Nonequilibrium Statistical Mechanics, Springer-Verlag (1985).
[11] D. Belitz, T. R. Kirkpatrick and T. Vojta, Rev. Mod. Phys. 77, 579 (2005).
[12] M. Bolsterli, M. Rich, and W. M. Visscher, Phys. Rev. A 41086 (1970).
[13] L. V. Keldysh, Zh. Eksp. Teor. Fiz. 47, 1515 (1964) Sov. Phys JETP 20, 235 (1965); R. P. Feynman and F. L. Vernon, Ann. Phys. 24, 118 (1963), A. Caldeira and A. Legget, Phys Rev. A 31, 1059 (1985).


[^0]:    *Department of Mathematics and Computer Science, Eindhoven University, P.O. Box 513 5600 MB Eindhoven, The Netherlands, c.giardina@tue.nl
    ${ }^{\dagger}$ CNRS-ESPCI, rue Vauquelin 10, 75231 Paris, France, jorge@pmmh.espci.fr

[^1]:    ${ }^{1}$ And in the quantum generalization of the present work, the twist will act on the closed time path action, involving twice as many fields, and not on the original Hamiltonian.

