Adiabatic Charge Pumping in Open Quantum Systems

JOSEPH E. AVRON
Technion

ALEXANDER ELGART
Courant Institute

GIAN MICHELE GRAF
ETH Hönggerberg

LORENZO SADUN
University of Texas at Austin

AND

KAI SCHNEE
California Institute of Technology

Abstract

We introduce a mathematical setup for charge transport in quantum pumps connected to a number of external leads. It is proven that under the rather general assumption on the Hamiltonian describing the system, in the adiabatic limit, the current through the pump is given by a formula of Büttiker, Prêtre, and Thomas, relating it to the frozen S matrix and its time derivative. © 2004 Wiley Periodicals, Inc.

1 Introduction

Transport in quantum pumps has been investigated in relation to various properties and from many perspectives [1, 7, 8, 15, 17, 21]. The goal of this article is to provide a rigorous setting for a single but important aspect of these devices, namely, the charge transport or, more precisely, its expectation value. The idealized setting is as follows: a pump, whose internal configuration varies slowly in time in a prescribed manner, is connected to n leads, or channels, along each of which independent electrons can enter or leave the pump. We assume that the electron in the lead has no transverse or spin degrees of freedom and may be thought of as a (nonrelativistic) particle moving on a half-line.[1] The incoming electron distribution, at zero temperature, is a Fermi sea with Fermi energy μ common to all leads. As a rule, this does not apply to the distribution of the outgoing electrons, as their energies may have been shifted while scattering at the pump. Because of this

[1] Such extra degrees of freedom can be represented by adding channels. In general, the different channels may then have different propagation speeds.

Communications on Pure and Applied Mathematics, Vol. LVII, 0528–0561 (2004)

imbalance, a net current is flowing in the leads. The expected charge transport is expressed by the formula [7, 8]

$$dQ_j = \frac{e}{2\pi}(\mathrm{i}(dS)S^*)_{jj}\,. \tag{1.1}$$

Here $S = (S_{ij})$ is the $n \times n$ scattering matrix at energy μ computed as if the pump were *frozen* into its instantaneous configuration. A change of the configuration is accompanied by a change $S \to S + dS$ of the scattering matrix and by a net charge dQ_j leaving the pump through lead j. Finally, e is the electron charge, which is henceforth set equal to 1.

We shall next present a mathematical framework in which (1.1) can be phrased as a theorem.

- The *single-particle Hilbert space* is given as

$$\mathcal{H} = \mathcal{H}_0 \oplus L^2\big(\mathbb{R}_+, \mathbb{C}^n\big)\,, \tag{1.2}$$

  where states in $L^2(\mathbb{R}_+, \mathbb{C}^n) = \bigoplus_{j=1}^n L^2(\mathbb{R}_+)$, respectively, in $\mathcal{H}_0$, describe an electron in one of the leads $j = 1, 2, \ldots, n$, respectively, in the pump proper. The latter Hilbert space is not further specified, but hypothesis (A2) below confers on the pump the role of an abstract finite box [23]. Let $\Pi_j : \mathcal{H} \to \mathcal{H}$ denote the projection onto $\mathcal{H}_0$ for $j = 0$ and on the j^{th} copy of $L^2(\mathbb{R}_+)$ for $j = 1, 2, \ldots, n$.
- Since the pump configuration is supposed to change slowly in time t, we will eventually consider the evolution of the electrons in an adiabatic limit, where $s = \varepsilon t$ is kept fixed as $\varepsilon > 0$ tends to 0. In terms of the rescaled time coordinate s, called *epoch*, the propagator $U_\varepsilon(s, s')$ on $\mathcal{H}$ satisfies the nonautonomous Schrödinger equation

$$\mathrm{i}\partial_s U_\varepsilon(s, s') = \varepsilon^{-1} H(s) U_\varepsilon(s, s')\,, \tag{1.3}$$

  where $H(s)$ is a family of self-adjoint *Hamiltonians* on $\mathcal{H}$ enjoying the following properties:

(A1)	$H(s) - H(s')$	is bounded and smooth in s,
(A2)	$\\|(H(s) + \mathrm{i})^{-m}\Pi_0\\|_1 < C$	for all s and some $m \in \mathbb{N}$,
(A3)	$H(s)\psi = -\dfrac{d^2\psi}{dx^2}$	for $\psi \in C_0^\infty\big(\mathbb{R}_+, \mathbb{C}^n\big)$,
(A4)	$\sigma_{\mathrm{pp}}(H(s)) \cap (0, \infty) = \varnothing$,	
(A5)	$H(s) = H_-$	for $s \le 0$.

  Here $\|\cdot\|_1$ denotes the trace class norm over $\mathcal{H}$, while the operator norm will be written as $\|\cdot\|$. Assumption (A3) states that a particle moving in a lead is free;

in particular, together with (A1), it implies that changes in the Hamiltonian are confined to the pump proper:

$$H(s) - H(s') = (H(s) - H(s'))\Pi_0 \,. \tag{1.4}$$

Assumption (A4) requires that there be no positive embedded eigenvalues; (A5) states that the pump is at rest for $s \le 0$.

- The state of the electrons should be at equilibrium as long as the pump is at rest. In particular, no net current ought yet to flow in that regime. This is achieved thanks to assumption (A5) by positing that the initial *1-particle density matrix* at some (and hence any) epoch $s_- < 0$ is of the form $\rho(H_-)$, where $\rho(\lambda)$ is a function of bounded variation with $\operatorname{supp} d\rho \subset (0, \infty)$. A good example is the Fermi sea, where $\rho(\lambda) = \theta(E - \lambda)$. The time evolution then acts as

$$\rho(H_-) \mapsto U_\varepsilon(s, s_-)\rho(H_-)U_\varepsilon(s_-, s) \,. \tag{1.5}$$

- We define a generator of exterior scaling with respect to (1.2) by

$$A = 0 \oplus \frac{1}{2\mathrm{i}}\left(\frac{d}{dx}v(x) + v(x)\frac{d}{dx}\right), \tag{1.6}$$

where $v(x) : [0, \infty) \to \mathbb{R}$ is smooth with $v(x) = 0$ for x small and $v(x) = x$ for x large and $v'(x) \ge 0$ everywhere. We note that $A = A^*$ commutes with Π_j, and set $A_j = A\Pi_j$. Basically, the operator A weighs the momentum $-\mathrm{i}d/dx$ of the particle, which can be of either sign, with its distance $x > 0$ from the pump. It therefore distinguishes between *incoming* and *outgoing* states, respectively, associated with spectral subspaces $A < -a$ and $A > a$ with some large $a > 0$. Detection of a particle, and hence of its charge, deep inside lead j may be realized as the operator $Q_j(a) = f(A_j - a) + f(-A_j - a)$, where $f \in C^\infty(\mathbb{R})$ is a switch function: $f(\alpha) = 0$ for $\alpha < -1$ and $f(\alpha) = 1$ for $\alpha > 1$. The *current operator* then consistently is

$$I_j(a) = \mathrm{i}[H(s), f(A_j - a) + f(-A_j - a)] =: I_{j+}(a) + I_{j-}(a) \,. \tag{1.7}$$

(In what follows, we shall sometimes suppress the index j for the sake of notational simplicity.) One feature of this choice of current operator is that the "ammeter" is located not at a fixed distance from the pump, but rather at a fixed number a of wavelengths from it: the longer the wavelength the more distant the "ammeter." In the case that one focuses on a narrow energy interval, say, near the Fermi energy, the ammeter is also at essentially a fixed distance from the pump.

We remark that by the support property of v and by (A3), the above commutator does not depend on s. The expectation value of the current at epoch s, i.e., in the state (1.5), is then given as

$$\langle I\rangle_j(s, a, \varepsilon) = \operatorname{tr}(U_\varepsilon(s, s_-)\rho(H_-)U_\varepsilon(s_-, s)I_j(a)) \,. \tag{1.8}$$

In contrast to $Q_j(a)$, which clearly has an infinite expectation value in that state, $I_j(a)$ is inclined to have a finite one. Moreover, it should behave as ε if,

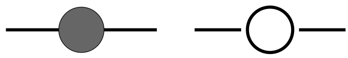

FIGURE 1.1. A scatterer with two channels (left) and its disconnected analogue (right). Neumann boundary conditions are imposed at the edges of the channels.

in accordance with (1.1), the charge dQ_j transferred during $ds = \varepsilon^{-1}dt$ is to have a nontrivial limit as $\varepsilon \to 0$.

Other realizations of the current operator are possible,[2] for instance,

$$\mathrm{i}[H(s), f(x_j - a)]\,,$$

or the example based on the precession of a spin proposed in [17], and the result (1.1) should be independent of the choice. Our definition (1.7) has the property that $I_j(a)$ splits naturally into two parts distinguished by their Heisenberg dynamics $U_\varepsilon(s_-, s)I_{j\pm}(a)U_\varepsilon(s, s_-)$: the incoming current $I_{j-}(a)$, which is essentially free in the past $s_- < s$ of the measurement epoch s, and the outgoing current $I_{j+}(a)$, which is free in the future. As the initial condition is set in the past of the measurement, only $I_{j+}(a)$ will be affected by scattering.

- Finally, we ought to state the reference dynamics H_0 to which $H(s)$ is compared in the (frozen) *scattering operator*

$$S(s) = S(H(s), H_0)\,. \tag{1.9}$$

We refer to [20, 25] for its definition, but recall that given a Hamiltonian H whose trajectories evolve according to H_0 at large times, i.e.,

$$\mathrm{e}^{-\mathrm{i}Ht}\psi = \mathrm{e}^{-\mathrm{i}H_0t}\psi_\pm + \mathrm{o}(1)\,, \quad t \to \pm\infty\,,$$

the scattering operator maps past to future asymptotes: $\psi_+ = S(H, H_0)\psi_-$. Since it commutes with H_0, it admits a direct integral representation over energies $E > 0$ in the spectrum of H_0, whose fibers $S(s, E)$, called *scattering matrices*, appear in (1.1). While the choice of H_0 is irrelevant to some extent, for the sake of simplicity let H_0 be the Laplacian, acting on $L^2(\mathbb{R}_+, \mathbb{C}^n)$, with a Neumann boundary condition at $x = 0$. $S(s, k^2)$, $k > 0$, then agrees with the familiar definition based on generalized eigenfunctions incident through lead i: $(\delta_{ji}\mathrm{e}^{-\mathrm{i}kx} + S_{ji}\mathrm{e}^{\mathrm{i}kx})_{j=1}^n$. In particular, this reproduces the standard form of the scattering matrix of two channels:

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

[2] The canonical choice of the current operators one normally finds in textbooks corresponds to $f(x) = \theta(x)$.

with r and r' the right and left reflection amplitudes, respectively, and t and t' the corresponding transmission amplitudes.

The fundamental equation (1.1) may thus be given the following reformulation:

$$\lim_{a\to\infty}\lim_{\varepsilon\to 0}\varepsilon^{-1}\langle I\rangle_j(s,a,\varepsilon) = -\frac{\mathrm{i}}{2\pi}\int_0^\infty d\rho(E)\left(\frac{dS}{ds}S^*\right)_{jj}. \tag{1.10}$$

In particular, for the Fermi sea $\rho(H_-) = \theta(\mu - H_-)$ as initial state, we recover (1.1) from $d\rho(E) = -\delta(E-\mu)dE$. The limit $a \to \infty$ is taken so as to have the current measurement made well outside of the scattering region, but after the adiabatic limit $\varepsilon \to 0$. By doing so, a current is still measured within the same epoch as the scattering process that generated it, though at a different time.

The result can be proven essentially in this form, though some problems that arise both in the infrared and the ultraviolet have to be dealt with. In fact, the adiabatic limit is realized [5] in the regime where the dimensionless quantity given by ε times the dwelling time of an electron in the pump is small. Low-energy particles have a large dwell time in the pumps and, in addition, may get trapped indefinitely as new bound states are born at the threshold $E = 0$. This means that no scattering description in terms of a single epoch is adequate at low energies. Similarly, at high energies resonances may become increasingly sharp with correspondingly long dwelling times.[3] On the other hand, low and high energy states do not contribute to the net current, since they are filled and empty, respectively, in both the incoming and the outgoing flow. We shall therefore concentrate on the contribution to the current coming from states in any intermediate energy range, as selected by the function χ below.

THEOREM 1.1 *Let $\chi \in C_0^\infty(0,\infty)$ with $\chi = 1$ on* $\operatorname{supp} d\rho$. *Redefine the current operator* (*with a UV and IR cutoff*)

$$I_{j,\pm}(s,a) = \chi(H(s))\mathrm{i}[H(s), f(\pm A_j - a)]\chi(H(s)), \quad a > 1, \tag{1.11}$$

in (1.7). *Then*

$$\lim_{a\to\infty}\lim_{\varepsilon\to 0}\varepsilon^{-1}\langle I\rangle_j(s,a,\varepsilon) = -\frac{\mathrm{i}}{2\pi}\int_0^\infty d\rho(E)\left(\frac{dS}{ds}S^*\right)_{jj}, \tag{1.12}$$

where $S = S(s,E)$. The double limit is uniform in $s \in I$, I being a compact interval, whence it carries over to the transferred charge

$$\int_0^{s/\varepsilon} dt'\langle I\rangle_j(\varepsilon t', a, \varepsilon) = \varepsilon^{-1}\int_0^s ds'\langle I\rangle_j(s', a, \varepsilon).$$

REMARK The auxiliary objects v and f affect the current operator. Nevertheless, they disappear from its expectation value in the adiabatic and the large a limits. This may be phrased as the statement that different ammeters measure the same current.

[3] If the pump is a chaotic billiard, the classical dynamics will, in general, have arbitrarily long periodic orbits. It is natural to expect that such orbits give rise to resonances.

We first give a heuristic derivation of equation (1.12), which may however serve as a guide through the complete proof. (For more hints, see [5].) One could argue that for computing the expectation values of observables, which, like $I_{j,-}(s,a)$, pertain to the incoming part of phase space, scattering may be ignored; that is, one may pretend that the state of the system at epoch s simply is $\rho(H(s))$. On the other hand, when discussing $I_{j,+}(s,a)$, one should do as if the state were

$$\rho(H(s)) + \varepsilon\big[S^{(1)}(s), \rho(H(s))\big] + \cdots \,, \tag{1.13}$$

where

$$S^{(1)}(s) = -\mathrm{i}\int_{-\infty}^{\infty} dt\, t\mathrm{e}^{\mathrm{i}H(s)t}\dot{H}(s)\mathrm{e}^{-\mathrm{i}H(s)t} \,. \tag{1.14}$$

This comes from linearizing the Hamiltonian $H(s+\varepsilon t) = H(s) + \varepsilon\dot{H}(s)t + \cdots$ around epoch s, since $U = 1 + \varepsilon S^{(1)}(s) + \cdots$ is then the propagator from $t = -\infty$ to $t = \infty$ in the interaction picture based on $H(s)$. Now (1.13) is the state $U\rho(H(s))U^*$ after scattering. The contribution of the first term there to $\langle I\rangle_{j,+}$ cancels against $\langle I\rangle_{j,-}$; see Lemma 2.2. The contribution of the second term is responsible for the right-hand side of equation (1.12). To foreshadow this outcome, we formally rewrite it (see Lemma 5.4) as

$$[S^{(1)}(s), \rho(H(s))] = -\mathrm{i}\partial_{s'}S(s', s)_{s'=s}\rho'(H(s)) \,, \tag{1.15}$$

with

$$\partial_{s'}S(s', s)_{s'=s} = -\mathrm{i}\int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H(s)t}\dot{H}(s)\mathrm{e}^{-\mathrm{i}H(s)t} \,. \tag{1.16}$$

Here, $1 + (s'-s)\partial_{s'}S(s', s)_{s'=s} + \cdots$ is the Born approximation for the scattering matrix $S(s', s)$ for the pair of autonomous Hamiltonians $H(s')$ and $H(s)$. The importance of equation (1.15) is twofold. First, it reduces matters to "frozen" scattering data and their derivatives. Second, it makes it clear why only the variation $d\rho(E)$ matters and, in particular, why for the Fermi sea $\rho(\lambda) = \theta(\mu - \lambda)$ only states at the Fermi energy μ contribute to the current.

Let us next discuss some of the conceptual issues involved in this result.

(1) Theorem 1.1 plays the role of the Kubo formula and like it gives a handle on transport, including dissipative transport, using Hamiltonian evolution. A well-known weakness of linear response theory, stressed by van Kampen [24], is that it takes the limit of linear response first and only then the thermodynamic limit. The correct order is, of course, the reverse. Theorem 1.1 is free of this criticism in that one starts with a system that has infinite extent, for which it is nevertheless possible to estimate the error made by linearizing the dynamics; see Lemma 4.1. The reason for that is the finite extent of the pump or, more precisely, the finite dwell times.

(2) Theorem 1.1 is an example of an adiabatic theorem for open, gapless systems. In contrast to other results of that kind, such as [3, 6], which establish that

an embedded eigenstate evolves adiabatically, ours is about the evolution associated with an infinite-dimensional spectral subspace, e.g., the Fermi sea. Moreover, the goal is not to establish that a spectral subspace is preserved by the dynamics; rather, it is to determine the amount by which it mingles with its complement, and the current is a measure thereof.

(3) On the left-hand side of (1.12) the scattering process and the measurement of the current are described as a single quantum history. This should be contrasted to usual textbook treatments of scattering rates, which have the following features: (i) The rates are computed classically as the product of a quantum mechanical scattering cross section and of an incident current; and (ii) the use of the scattering cross section tacitly replaces the actual state by its free asymptote. For a static potential and a steady beam, both steps have been justified [12] in the limit where the measurement is deferred all the way to $t \to \infty$. This is not quite so in the present fluctuating setting, where the ammeter is located at an intermediate scale, as specified by the order of the ε and a limits: far away from the pump on the scale of the scatterer, but close to it on the scale of the distance traveled by a particle on the adiabatic time scale.

(4) The formula of Büttiker et al., equation (1.1), is pointwise in time. Suppose we represent the flow by means of coherent states of widths ΔE and Δt. In line with the remark just made, one might suspect that Δt needs to be picked small with respect to the adiabatic time scale ε^{-1}, and hence $\Delta E \gtrsim \hbar\varepsilon$ by the Heisenberg uncertainty relation. At temperature β^{-1} the 1-particle distribution of the incoming flow is $(1 + e^{\beta(E-\mu)})^{-1}$, which suggests that $\Delta E \lesssim \beta^{-1}$. This seemingly presents an obstacle to applying scattering arguments when $\beta^{-1} < \hbar\varepsilon$. Our result, which applies to $\rho(\lambda) = \theta(\mu - \lambda)$, shows that this obstacle can be overcome, and that one *can* take the zero temperature limit $\beta \to \infty$ before taking $\varepsilon \to 0$.

(5) The trace with respect to j of equation (1.1) bears a close relation to the Birman-Krein formula [25] $\det S(s, E) = \mathrm{e}^{-2\pi \mathrm{i}\xi(s,E)}$, where the spectral shift $\xi(s, E)$ represents the deficiency of particles in the Fermi sea of $H(s)$ as compared to that of H_0. More precisely, equation (1.1) is a dynamical complement to that formula, inasmuch it states that the total charge $\sum_{j=1}^{n} dQ_j = d\xi$ emitted from an adiabatically operated pump matches the parametric change of the charge inside.

Results related to Theorem 1.1 have been obtained at the level of both physical and mathematical rigor. Among the former we mention, besides [4, 7, 8], the formula of Lee, Lesovik, and Levitov [17], which expresses the noise generated by quantum pumps (as well as other moments) in terms of the scattering data. However, the relations regarding noise are not local in time. Rather these are integral relations that hold for a cycle of the pump. Physically, what sets the current apart from the noise is its linear dependence on ρ. Rigorous mathematical description of the adiabatic scattering of wave packets is discussed in [18, 19]. Like our result, they rely on propagation estimates.

The plan of the rest of the paper is as follows: In Section 2 we shall verify that $\langle I\rangle_j(s,a,\varepsilon)$ and the Stieltjes integral in (1.12) are well-defined. Further preliminaries, like propagation estimates, will be addressed in Section 3. In Section 4 we shall compute the limit $\varepsilon \to 0$ of the current in terms of data involving $H(s)$ and $\dot H(s)$, but oblivious of the past $\{H(t)\}_{t<s}$. The expression will further reduce to the "frozen" scattering data (1.9) in Section 5 where the limit $a \to \infty$ is taken. In the appendix we establish some trace class estimates for operators related to (1.11). The main ideas are further discussed at the beginning of Sections 4 and 5.

We conclude with a remark on notation. Multiple commutators are denoted by $\mathrm{ad}_A^{(k)}(B) = [\mathrm{ad}_A^{(k-1)}(B), A]$ with $\mathrm{ad}_A^{(0)}(B) = B$. By $F(A \geq a)$ we mean the spectral projection of A onto $[a,\infty)$. The trace class ideal is denoted as $\mathcal{J}_1$. Generic constants are indicated by C. The limit in the strong operator topology is written as s-lim.

2 The Current Operator and the Scattering Matrix

The state of independent quantum particles is described by a density matrix $0 \leq \rho$ normalized so that $\operatorname{tr}\rho$ is the number of particles. In the case of fermions, $\rho \leq 1$. Thermodynamic systems have $\operatorname{tr}\rho = \infty$ and observables that are otherwise innocent, and bounded operators in particular may fail to have finite expectation values. For example, the charge associated with the "box" $f(A-a)$ in phase space is infinite. Nevertheless, the current flowing into the box should have a finite expectation. We begin by showing that the incoming and outgoing current operators of equation (1.7) are trace class and consequently, the expectation value $\langle I\rangle_j(s,a,\varepsilon)$ in any fermionic state is well-defined.

A classical interpretation of the trace class condition is for the observable to be associated with a localized (bounded) function in phase space. The heuristic reason why the current is trace class is then as follows: The commutator $[H(s), f(A_j - a)]$ is localized near the boundary of the box, a curve (hyperbola) in phase space. This is where the ammeter is. The ultraviolet and infrared cutoff $\chi(H(s))$ then further delineates a compact region of phase space near the hyperbola. Our first preliminary result confirms this picture.

PROPOSITION 2.1 *The operator of incoming and outgoing current in the j^{th} channel, $I_{j\pm}(s,a)$, is a trace class operator which is localized near $\pm a$ in the sense that*

$$\|F(|A \mp a| \geq \alpha) I_{j\pm}(s,a)\|_1 \leq C_N (1+\alpha)^{-N} \quad \text{for all } N \in \mathbb{N},\ \alpha \geq 0. \tag{2.1}$$

PROOF: This proposition is a direct consequence of Lemma 3.3 below. □

The pumping formula of Theorem 1.1 implies that no current flows if the pump is not operating, since $dS/ds = 0$ if $H(s)$ is independent of s. Indeed, in the state $\rho(H(s))$, as in a thermal state, different leads are at equilibrium with one another; moreover, in each lead, right- and left-moving states yield compensating currents if equally occupied. When the pump is in operation, it will still prove useful to know that no persistent currents are flowing in the "adiabatic" state $\rho(H(s))$.

LEMMA 2.2 *The currents in the state* $\rho(H(s))$ *vanish, namely,*

$$\mathrm{tr}\big(\rho(H(s))(I_{j+}(s,a)+I_{j-}(s,a))\big)=0\,. \tag{2.2}$$

PROOF: We omit s from the notation. Since $I_\pm(a)\in\mathcal{J}_1$, it suffices to prove (2.2) for smooth ρ, since one may approximate the general case by a sequence $\text{s-lim}_{n\to\infty}\rho_n(H)=\rho(H)$.

First we show that $\mathrm{tr}(\rho(H)I_\pm(a))$ is independent of a. Note that $I_\pm(a_1)-I_\pm(a_2)=\chi(H)\mathrm{i}[H,g(A_j)]\chi(H)$ with $g(A_j)=f(\pm A_j-a_1)-f(\pm A_j-a_2)$. Since $\chi(H)g(A_j)=\chi(H)g(A)\Pi_j\in\mathcal{J}_1$, see (A.17), we have

$$\begin{aligned}\mathrm{tr}\big(\rho(H)(I_\pm(a_1)-I_\pm(a_2))\big)&=\\ &\mathrm{i}\,\mathrm{tr}(\rho\chi(H)Hg(A_j)\chi(H)-\rho\chi(H)g(A_j)H\chi(H))=0\end{aligned} \tag{2.3}$$

by cyclicity. It thus suffices to prove (2.2) in the limit as $a\to\infty$. To this end, let H_0 be the Neumann Hamiltonian on the leads introduced below equation (1.9), and let $J:L^2(\mathbb{R}_+,\mathbb{C}^n)\to\mathcal{H}$ be the embedding given by (1.2). We maintain that

$$\lim_{a\to\infty}\left\|(\rho(H)I_\pm(a)-J\rho(H_0)I^0_\pm(a)J^*\right\|_1=0\,, \tag{2.4}$$

where $I^0_\pm(a)$ is defined as in (1.11) with H replaced by H_0. Indeed, by expanding that commutator we reduce matters to two estimates, both of the form

$$\lim_{a\to\infty}\left\|\chi_1(H)f(\pm A_j-a)\chi_2(H)-J\chi_1(H_0)f(\pm A_j-a)\chi_2(H_0)J^*\right\|_1=0\,,$$

with $\chi_i\in C_0^\infty(\mathbb{R})$, $i=1,2$. Then we write the difference as

$$\begin{aligned}&\big(\chi_1(H)-J\chi_1(H_0)J^*\big)f(\pm A_j-a)\chi_2(H)\\ &\qquad+J\chi_1(H_0)J^*f(\pm A_j-a)\big(\chi_2(H)-J\chi_2(H_0)J^*\big)\,.\end{aligned}$$

Since $\chi_i(H)-J\chi_i(H_0)J^*\in J_1$ by (A.6) and $\text{s-lim}_{a\to\infty}f(\pm A_j-a)=0$, equation (2.4) follows. At this point we need only

$$\mathrm{tr}\big(\rho(H_0)(I^0_+(a)+I^0_-(a))\big)=0\,,$$

which holds by time reversal invariance: for $K\psi(x)=\bar{\psi}(x)$ we have $KH_0K=H_0$, $KAK=-A$, and hence $KI^0_\pm(a)K=-I^0_\mp(a)$. □

REMARK One can establish the result without explicitly using time reversal and using instead the pull-through formula equation (A.10).

Mourre theory (see, e.g., [2]) plays a double role in our analysis. First, it is at the heart of time-dependent scattering theory and the propagation estimates that we shall discuss in the next section. At the same time, the theory also plays a role in time-independent methods, and we shall use it to establish the differentiability of the scattering matrix that appears on the right-hand side of equation (1.12).

PROPOSITION 2.3 *Under assumptions* (A1)–(A5)*, the fibers of the frozen S matrix,* $S(s, E)$*, are continuously differentiable in s at* $E > 0$*. In particular, the integral on the right-hand side of equation* (1.12) *is well-defined for* ρ *with bounded variation.*

PROOF: The Hamiltonians $H(s)$ are dilation analytic of type (A) with respect to the conjugate operator A. In particular,

$$\mathrm{ad}_A^{(k)}(H) \quad \text{is } H(s)\text{-bounded.} \tag{2.5}$$

More importantly, for any energy $E > 0$ the Mourre estimate holds:

$$E_\Delta(H(s))\mathrm{i}[H(s), A]E_\Delta(H(s)) \geq \theta_0 E_\Delta(H(s)) \tag{2.6}$$

for some open interval $\Delta \ni E$ and $\theta_0 > 0$. Note that a compact term on the right-hand side can be dismissed by assumption (A4). The Mourre estimate (2.6) is stable under small bounded perturbations of s, which is seen from (A.5) and from the fact that $\mathrm{i}[H(s), A]$ is independent of s, just as is the commutator in (1.7). Therefore, (2.6) holds uniformly in $s \in I$ and $E \in J$, with $J \subset (0, \infty)$ compact, and so do the usual consequences of these assumptions. They include:

(i) *Resolvent smoothness*. Let $\langle A \rangle = (1 + A^2)^{1/2}$ and $r > \frac{1}{2}$. Then

$$B(z, s) = \langle A \rangle^{-r}(H(s) - z)^{-1}\langle A \rangle^{-r}$$

has smooth boundary values at $z = E + \mathrm{i}0$, $E \in J$, satisfying

$$\left\| \partial_E^k B(E + \mathrm{i}0, s) \right\| \leq C_k \tag{2.7}$$

for $k = 0, 1, \ldots$; see [16]. Since

$$\partial_s B(z, s) = -\langle A \rangle^{-r}(H(s) - z)^{-1}\dot{H}(s)(H(s) - z)^{-1}\langle A \rangle^{-r}$$

and $\dot{H}(s) = \langle A \rangle^{-r}\dot{H}(s)\langle A \rangle^{-r}$, the function $B(E + \mathrm{i}0, s)$ is jointly continuously differentiable in (E, s).

(ii) *H-smoothness*. $\langle A \rangle^{-r}$ is $H(s)$-smooth [20, 25] as a consequence of (2.7) for $k = 0$.

(iii) *Stationary representation of the scattering matrix.* Let

$$E_J(H(s))\mathcal{H} \to \int_J^{\oplus} \mathbb{C}^n dE\,, \qquad \psi \mapsto \{\psi(E)\}\,, \tag{2.8}$$

be the spectral representation for $H(s)$ on J, and set $\Gamma_0(E)\psi = \psi(E)$. Then $\Gamma_0(E)\langle A \rangle^{-r} : \mathcal{H} \to \mathbb{C}^n$ is bounded by (ii). Let $S(s', s)$ be the scattering operator for the pair $(H(s'), H(s))$. Its fibers $S(E) : \mathbb{C}^n \to \mathbb{C}^n$ with respect to (2.8) admit the representation [25]

$$S(E) = 1 - 2\pi\mathrm{i}\Gamma_0(\lambda)(V - V(H(s') - (E + \mathrm{i}0))^{-1}V)\Gamma_0(\lambda)^*\,, \tag{2.9}$$

with $V = H(s') - H(s)$. The right-hand side is defined pointwise because $V = \langle A \rangle^{-r}V\langle A \rangle^{-r}$ and because of (i). From this, equation (2.9), and the statements about $B(E + \mathrm{i}0, s)$, we see that $S(s', s)E_J(H(s))$ is continuously differentiable in $s' \in I$, and that the derivative can be computed fiberwise. The same applies to the scattering operator $S(s) = S(H(s), H_0)$, though (2.9) appears slightly modified. $\square$

3 Propagation Estimates

Propagation estimates play a key and multiple role in our analysis. One role is that they guarantee that particles do not get stuck in the pump. Consequently, the scattered particle indeed sees a frozen scatterer to lowest order in the adiabatic limit, and a linearly changing scatterer to first order. At the same time, propagation estimates also play a role in establishing that the current measured by the ammeter at epoch s is determined by the state of the pump at the same epoch, in the adiabatic limit. This may be interpreted as a statement that the particles neither linger nor disperse too badly in the channels.[4]

Propagation estimates play yet another role in establishing the "rigidity" of the current: the expectation value for the current a priori depends on a choice of a switch function f, the function $v(x)$ in the generator of dilation, and a choice of the initial configuration of the pump H_-. This dependence is suppressed from our notation because Theorem 1.1 implies that the dependence disappears in the limit. Ultimately, this independence is a consequence of propagation estimates.

Equation (2.6) implies a minimal escape velocity estimate [11, 14] for the autonomous dynamics generated by $H(s)$. The constants involved are understood as being uniform in $s \in I$ and in the stated range for a. Within proofs we shall abbreviate $H \equiv H(s)$.

LEMMA 3.1 *Let χ in $C_0^\infty(0,\infty)$ (in particular, with support away from $E = 0$). Then, for some $\theta > 0$, for all $a \in \mathbb{R}$, $b, t \geq 0$, and $N \in \mathbb{N}$,*

$$\left\| F(A \leq a - b + \theta t) \mathrm{e}^{-\mathrm{i}H(s)t} \chi(H(s)) F(A \geq a) \right\| \leq C_N(\theta)(b + \theta t)^{-N} . \tag{3.1}$$

Similarly, if $b, t < 0$, then

$$\left\| F(A \geq a - b + \theta t) \mathrm{e}^{-\mathrm{i}H(s)t} \chi(H(s)) F(A \leq a) \right\| \leq C_N(\theta)|b + \theta t|^{-N} . \tag{3.2}$$

PROOF: The case of $b = 0$ is covered by theorem 1.1 in [14], since its hypothesis (besides (2.6)) that $\mathrm{ad}_A^{(k)}(f(H))$ is bounded for $f \in C_0^\infty(\mathbb{R})$ and $k \geq 1$ holds true by (2.5). To be precise, the result is formulated there for $\operatorname{supp}\chi \subset \Delta$, where Δ is as in (2.6) and $0 < \theta < \theta_0$, but it extends to our case by a covering argument. Actually, the proof given there essentially covers the general case $b \neq 0$.

More precisely, let

$$A_{t\tau} = \tau^{-1}\left(A - a + \frac{b}{2} - \theta_0 t\right)$$

and $f \in C^\infty(\mathbb{R})$ be a function with $|f^{(k)}(x)| \leq C\langle x\rangle^{-k}$, $f' \leq 0$, and $f(x) = 0$ for $x \geq 0$. Then

$$\left\| f(A_{t\tau}) \mathrm{e}^{-\mathrm{i}Ht} \chi(H) F(A \geq a) \right\| \leq C_N \tau^{-N}$$

[4] Dispersion arises because we use a nonrelativistic (quadratic) kinetic energy in the leads. In much of the literature on pumps, dispersion is circumvented by making the kinetic energy linear in the momentum.

uniformly in $0 \le t \le \tau$ and $a \in \mathbb{R}$. For $b = 0$, this is equation (2.11) in [14], whose proof applies to $b \ge 0$ as well.

Let $\tau = b + t$. Since
$$\frac{b-\theta t}{b+t} \ge \frac{b/2-\theta_0 t}{b+t} + \delta$$
for some $\delta > 0$ and all $b, t \ge 0$, we have
$$F(A \le a - b + \theta t) \le F\left(\frac{A - a + (b/2) - \theta_0 t}{b+t} \le -\delta\right) \le f(A_{t\tau})$$
for some f of the required type. □

Lemma 3.3 below is a refined version of Proposition 2.1 above. The discussion is simplified by the observation that the regularized currents equation (1.11) may be written as

$$I_{j\pm}(s,a) = \chi(H(s))\mathrm{i}[H_b(s), f(\pm A_j - a)]\chi(H(s))\,, \tag{3.3}$$

where $H_b(s) = H(s)b(H(s))$ with $b \in C_0^\infty(\mathbb{R})$ and $b\chi = \chi$. The unregularized current, equation (1.7), is independent of s by (A3) and the commutation $[H(s), \Pi_j] = 0$. Since the commutation fails when $H(s)$ is replaced by $H_b(s)$, the regularized current is a priori epoch dependent. However, the commutation is essentially recovered on the "box" $f(\pm A - a)$ when a is large. More precisely, we have the following:

LEMMA 3.2 *For $j = 0, 1, \dots, n$ and $a \ge -1$, we have*

$$\left\|[H_b(s), \Pi_j] f(\pm A - a)(\pm A - a + \mathrm{i})^2\right\| \le C\,. \tag{3.4}$$

PROOF: Since $(A+\mathrm{i})^{-2} f(\pm A - a)(\pm A - a + \mathrm{i})^2$ is uniformly bounded in $a \ge 1$, we may prove instead that

$$\left\|[H_b(s), \Pi_j](A + \mathrm{i})^2\right\| \le C\,. \tag{3.5}$$

We begin by showing that $\Pi_i H_b \Pi_j (A+\mathrm{i})^2 = \Pi_i H_b \Pi_j (A_j + \mathrm{i})^2$ is bounded for $i \ne j$. Indeed,
$$H_b(A_j+\mathrm{i})^2 = (A_j+\mathrm{i})^2 H_b + 2(A_j+\mathrm{i})[H_b, A_j] + [[H_b, A_j], A_j]\,,$$
from which we infer that $(A_j+\mathrm{i})^{-2} H_b (A_j + \mathrm{i})^2$ is bounded. Hence so is (use $\Pi_i A_j = 0$)
$$\Pi_i H_b \Pi_j (A_j + \mathrm{i})^2 = -\Pi_i (A_j+\mathrm{i})^{-2} H_b (A_j+\mathrm{i})^2 \Pi_j\,.$$
Now, setting $\bar{\Pi}_j = 1 - \Pi_j = \sum_{k=0,k\ne j}^n \Pi_k$, we have
$$[H_b, \Pi_j](A+\mathrm{i})^2 = \left(\bar{\Pi}_j H_b \Pi_j - \Pi_j H_b \bar{\Pi}_j\right)(A+\mathrm{i})^2\,,$$
and the result follows. □

This implies that although the regularized current operator a priori depends on the epoch and the pump, the dependence disappears in the limit of large a.

LEMMA 3.3

$$\left\| \mathrm{i}[H_b(s),\, f(\pm A_j - a)]\chi(H(s)) \right\|_1 \le C\,, \tag{3.6}$$

$$\left\| F(A < \pm a - \alpha)\mathrm{i}[H_b(s),\, f(\pm A_j - a)]\chi(H(s)) \right\|_1 \le C_N(1+\alpha)^{-N}\,, \tag{3.7}$$

$$\left\| F(A > \pm a + \alpha)\mathrm{i}[H_b(s),\, f(\pm A_j - a)]\chi(H(s)) \right\|_1 \le C_N(1+\alpha)^{-N}\,, \tag{3.8}$$

for $a, \alpha \ge 1$. *The same bounds hold in the operator norm if* $\chi(H(s))$ *is replaced with* $(\pm A - a + \mathrm{i})^2$.

Estimate (3.8) prevents the current operators from being located very far in the outgoing region of phase space. This will play a role in the next lemma and in Section 4. Actually, instead of $(3.8)_-$, we shall use there the weaker statement with characteristic function $F(A > a+\alpha)$. The pair $(3.7)_+$ and $(3.8)_-$ keeps the current operators away from the pump, a property used in Section 5.

PROOF: The estimates to be proven are of the form

$$\begin{aligned} &\|T[H_b,\, f(\pm A_j - a)]\chi(H)\|_1 \\ &\quad \le \left\| T[H_b,\, f(\pm A_j - a)](\pm A - a + \mathrm{i})^2 \right\| \left\| (\pm A - a + \mathrm{i})^{-2}\chi(H) \right\|_1 \\ &\quad \le C \left\| T[H_b,\, f(\pm A_j - a)](\pm A - a + \mathrm{i})^2 \right\|\,, \end{aligned} \tag{3.9}$$

where we have used (A.16).

We then have to establish the corresponding bounds for the remaining operator norm. Since $g(A_j) = g(0) + (g(A) - g(0))\Pi_j$, we have

$$f(\pm A_j - a) = f(\pm A - a)\Pi_j$$

due to $f(-a) = 0$ for $a > 1$. Writing $f = f\tilde{f}$, where $\tilde{f}(\,\cdot\,) = f(\,\cdot\, + 2)$, the commutator in (3.9) is

$$\left[H_b,\, f\Pi_j\tilde{f}\right] = \left[H_b,\, f\right]\Pi_j\tilde{f} + f\Pi_j\left[H_b,\, \tilde{f}\right] + f\left[H_b,\, \Pi_j\right]\tilde{f}\,,$$

with $\tilde{f} = \tilde{f}(\pm A - a)$. In the contribution to (3.9) of the first two terms, the projections Π_j may be moved out to the right or to the left, using $[T, \Pi_j] = 0$. As for the last term, we use (3.4). At this point, (3.9) reduces to corresponding estimates for

$$\|T[H_b,\, f(A)](A + \mathrm{i})^2\| + \|Tf(A)\|\,, \tag{3.10}$$

where we replaced $\pm A - a$ by A, as the argument given below applies to the more general case.

In the case of (3.6), where $T = 1$, the second term (3.10) is clearly bounded. On the first term we use the commutator expansion (see [13, equation (B.16)] or

[10]), based on the Helffer-Sjöstrand representation of $f(A)$.

$$
\begin{aligned}
[H_b, f(A)] &= \sum_{k=1}^{m-1} \frac{1}{k!}(-1)^{k-1} \operatorname{ad}_A^{(k)}(H_b) f^{(k)}(A) + R_m\,, \\
R_m &= -\frac{1}{\pi} \int dx\, dy \partial_{\bar z} \tilde f(z)(A-z)^{-1} \operatorname{ad}_A^{(m)}(H_b)(A-z)^{-m}\,,
\end{aligned}
\tag{3.11}
$$

where $\partial_{\bar z} = (\partial_x + \mathrm{i}\partial_y)/2$ and $\tilde f$ is an almost-analytic extension of f, which may be chosen in such a way that

$$
\int dx\, dy |\partial_{\bar z} \tilde f(z)||y|^{-p-1} \le C \sum_{k=0}^{m+2} \|f^{(k)}\|_{k-p-1}
$$

for $p = 0, 1, \ldots, n$, the norms being defined as $\|f\|_k = \int dx \langle x\rangle^k |f(x)|$. The choice of [13] is such that if $\operatorname{supp} f'$ is compact, as it is in our case, then $|y| \ge C_1|x| - C_2$, $C_1, C_2 > 0$, for $z = x + \mathrm{i}y \in \operatorname{supp} \tilde f$, which thus implies

$$
\|(A-z)^{-1}(A+\mathrm{i})\| \le C(|y|^{-1} + 1)\,. \tag{3.12}
$$

The expanded terms remain bounded if multiplied by $(A+\mathrm{i})^2$ from the right. For the remainder we obtain

$$
\left\|R_m(A+\mathrm{i})^2\right\| \le C \left\|\operatorname{ad}_A^{(m)}(H_b)\right\| \sum_{k=0}^{m+2} \left(\|f^{(k)}\|_{k-m-1} + \|f^{(k)}\|_{k-m+1}\right), \tag{3.13}
$$

which is finite for $m \ge 3$.

We shall next prove (3.7) with $F(A < -\alpha)$ replaced by $F(A < -3\alpha)$ for ease in notation below. This may be further replaced by $f(-\alpha^{-1}A - 2)$ because $F(A < -3\alpha) = F(A < -3\alpha) f(-\alpha^{-1}A - 2)$. Since $f(-\alpha^{-1}A - 2) f(A) = 0$, the claim equation (3.10) reads

$$
\left\|[H_b, f(-\alpha^{-1}A - 2)] f(A)(A+\mathrm{i})^2\right\| \le C_N \alpha^{-N}\,. \tag{3.14}
$$

We now apply the expansion (3.11) to $-\alpha^{-1}A - 2$ instead of A. Because

$$
f^{(k)}(-\alpha^{-1}A - 2) f(A) = 0\,,
$$

only the remainder contributes. To bound $\|R_m(A+\mathrm{i})^2\|$ we use

$$
\left\|\left(-\alpha^{-1}A - 2 - z\right)^{-1}(A+\mathrm{i})\right\| \le C\alpha\left(|y|^{-1} + 1\right)
$$

instead of (3.12) and collect the powers of α^{-1} generated by each commutator. We thus obtain the bound of (3.13) times α^{-m+2}.

Finally, (3.8) can be brought into a form similar to (3.7) by replacing f with $f - 1$. Both functions have the same commutator with H_b but essentially complementary supports. □

In Section 4 we shall describe the dynamics (1.3) in terms of the autonomous dynamics generated by the Hamiltonians $H(s)$. Once this is achieved, the choice of an argument in initial 1-particle density matrix ρ, be it H_- or $H(s)$, does not matter much for the current measurement, as defined by (1.11). This is the content of the following lemma:

LEMMA 3.4 *Let ρ and χ be as in Theorem* 1.1. *Then, for $a \geq 1$,*

$$\lim_{t\to-\infty} \left\| (\rho(H(s)) - \rho(H_-))\mathrm{e}^{-\mathrm{i}H(s)t} I_\pm(s,a) \right\|_1 = 0\,. \tag{3.15}$$

We remark that no claim of uniformity with respect to s and a is made here. The statement for $t \to +\infty$ is also true, but not needed.

PROOF: We first consider the case where ρ is smooth, and since H is bounded below, we may assume $\rho \in C_0^\infty(\mathbb{R})$. Then

$$\rho(H) - \rho(H_-) \in \mathcal{J}_1 \tag{3.16}$$

by equation (A.5). To estimate the trace norm in (3.15), we use (3.3), insert

$$1 = F(A \leq a+\alpha) + F(A > a+\alpha)$$

to the left of the commutator in (1.11), and use (3.6) and (3.8). We thus obtain the bound

$$\|(\rho(H) - \rho(H_-))\mathrm{e}^{-\mathrm{i}Ht}\chi(H)F(A \leq a+\alpha)\| \cdot C + C_N\alpha^{-N}\,. \tag{3.17}$$

The remaining operator norm is bounded for $t \leq 0$ by

$$\|(\rho(H) - \rho(H_-))F(A \leq a+\alpha+\theta t)\| + C_N t^{-N}\,, \tag{3.18}$$

where we used (3.2) with $b = 0$. We pick $\alpha = -\theta t/2$, so that the remainder in (3.17) tends to 0, and $\text{s-lim}_{t\to-\infty} F(\,\cdot\,) = 0$ in (3.18). Since $\rho(H) - \rho(H_-)$ is compact, the norm vanishes in the limit.

In the general case, where ρ is of bounded variation, let $\rho_n \in C_0^\infty(\mathbb{R})$, with $\sup_n \|\rho_n\|_\infty < \infty$, be a sequence such that $\rho_n(\lambda) \to \rho(\lambda)$ pointwise, whence $\text{s-lim}_{n\to\infty} \rho_n(H) = \rho(H)$, and the same for H_- instead of H. In addition,

$$\operatorname*{s-lim}_{t\to-\infty} \left(\mathrm{e}^{-\mathrm{i}Ht}P_{\mathrm{ac}}(H) - \mathrm{e}^{-\mathrm{i}H_-t}\Omega_-\right) = 0$$

by definition of the wave operator $\Omega_- = \Omega_-(H_-, H)$ [20, 25]. Since $I_\pm(s,a)$ is trace class by (3.6) and since

$$\operatorname*{s-lim}_{n\to\infty} X_n = 0\,, \quad Y \in \mathcal{J}_1 \Rightarrow \lim_{n\to\infty} \|X_nY\|_1 = 0\,, \tag{3.19}$$

we have

$$\begin{aligned}
\lim_{n\to\infty} \|(\rho_n(H) - \rho(H))I_\pm(s,a)\|_1 &= 0\,,\\
\lim_{n\to\infty} \|(\rho_n(H_-) - \rho(H_-))\Omega_- I_\pm(s,a)\|_1 &= 0\,,\\
\lim_{t\to-\infty} \left\|(\mathrm{e}^{-\mathrm{i}Ht} - \mathrm{e}^{-\mathrm{i}H_-t}\Omega_-)I_\pm(s,a)\right\|_1 &= 0\,,
\end{aligned} \tag{3.20}$$

where we dropped $P_{\mathrm{ac}}(H)$ due to $P_{\mathrm{ac}}(H)\chi(H) = \chi(H)$. We then estimate ($I_\pm \equiv I_\pm(s,a)$),

$$
\begin{aligned}
&\big\|(\rho(H) - \rho(H_-))\mathrm{e}^{-\mathrm{i}Ht} I_\pm\big\|_1 \\
&\quad \le \big\|(\rho(H) - \rho_n(H))\mathrm{e}^{-\mathrm{i}Ht} I_\pm\big\|_1 + \big\|(\rho_n(H) - \rho_n(H_-))\mathrm{e}^{-\mathrm{i}Ht} I_\pm\big\|_1 \\
&\qquad + \big\|(\rho_n(H_-) - \rho(H_-))(\mathrm{e}^{-\mathrm{i}Ht} - \mathrm{e}^{-\mathrm{i}H_-t}\Omega_-) I_\pm\big\|_1 \\
&\qquad + \big\|(\rho_n(H_-) - \rho(H_-))\mathrm{e}^{-\mathrm{i}H_-t}\Omega_- I_\pm\big\|_1 \\
&\quad \le \big\|(\rho(H) - \rho_n(H)) I_\pm\big\|_1 + \big\|(\rho_n(H) - \rho_n(H_-))\mathrm{e}^{-\mathrm{i}Ht} I_\pm\big\|_1 \\
&\qquad + C\big\|(\mathrm{e}^{-\mathrm{i}Ht} - \mathrm{e}^{-\mathrm{i}H_-t}\Omega_-) I_\pm\big\|_1 + \big\|(\rho_n(H_-) - \rho(H_-))\Omega_- I_\pm\big\|_1 .
\end{aligned}
$$

Given $\epsilon > 0$ we first pick n large enough such that the first and last terms together are less than $\epsilon/2$. For large negative t, the same is true for the second and third terms by (3.20) and the first part of the proof. □

4 The Adiabatic Limit

The current generated by adiabatic pumps can be understood within the general framework of the theory of linear response: the adiabatic limit corresponds to weak driving, and the formal derivation of equation (1.1) in [8] is a perturbation expansion. Formally, the change in the state ρ of a system, obtained by linearizing the Hamiltonian around epoch s, is

$$
\begin{aligned}
U_\varepsilon(s,s_-)\rho(H(s))U_\varepsilon(s_-,s) - \rho(H(s)) \approx \\
- \mathrm{i}\varepsilon \int_{-\infty}^{0} dt\, t\, \mathrm{e}^{\mathrm{i}H(s)t}\big[\dot H(s), \rho(H(s))\big]\mathrm{e}^{-\mathrm{i}H(s)t} .
\end{aligned}
\tag{4.1}
$$

One immediate difficulty with this expression is that the integrand on the right-hand side grows linearly with time. As an operator identity, the above equation does not make sense, and the right-hand side is not recognizably of order ε.

One of the reasons that a perturbation expansion can nevertheless be made is that the current of equation (1.11) has good localization in phase space and so distinguishes a region of phase space where ρ is to be evaluated. Therefore, only a restricted range of times contribute to the integral: the time associated with propagation from the pump to the ammeter. This makes the expectation value of the current well-defined. Estimates of this kind are known as propagation estimates and are controlled by Mourre theory.

In this section the limit $\varepsilon \to 0$ in (1.12) is taken as a is kept fixed. The main result is the following:

PROPOSITION 4.1 *For fixed $a \ge 1$, we have*

$$
\begin{aligned}
\lim_{\varepsilon\to 0} \varepsilon^{-1} \operatorname{tr}\big([U_\varepsilon(s,s_-)\rho(H_-)U_\varepsilon(s_-,s) - \rho(H(s))] I_\pm(s,a)\big) = \\
\operatorname{tr}\big([\Omega_-^{(1)}(s), \rho(H(s))] I_\pm(s,a)\big)
\end{aligned}
\tag{4.2}
$$

uniformly in $s \in I$, where

$$\Omega_-^{(1)}(s) = -\mathrm{i}\int_{-\infty}^{0} dt\, t\, \mathrm{e}^{\mathrm{i}H(s)t}\dot{H}(s)\mathrm{e}^{-\mathrm{i}H(s)t}\,. \tag{4.3}$$

Moreover,

$$\lim_{\varepsilon\to 0}\varepsilon^{-1}\,\mathrm{tr}\big(U_\varepsilon(s,s_-)\rho(H_-)U_\varepsilon(s_-,s)(I_+(s,a)+I_-(s,a))\big) = \mathrm{tr}\big([\Omega_-^{(1)}(s),\rho(H(s))](I_+(s,a)+I_-(s,a))\big)\,. \tag{4.4}$$

REMARKS

(i) The integral (4.3) is an integral that converges in the trace class norm once multiplied from the left or right by $I_\pm(s,a)$, as in (4.2).

(ii) Equation (4.2) separately describes, to leading order, the incoming and outgoing currents in an adiabatically evolved state as compared to the corresponding instantaneous state $\rho(H(s))$. Equation (4.4) is then an immediate consequence of (2.2).

(iii) $\Omega_-^{(1)}(s)$ is formally the first-order-in-ε term in the expansion of the wave operator, which for fixed s relates $U_\varepsilon(s',s)$ to the autonomous dynamics $u_s(s'-s)$ generated by the Hamiltonian $H(s)$:

$$u_s(\sigma) := \mathrm{e}^{-iH(s)\varepsilon^{-1}\sigma}\,,$$

where ε has been suppressed from the notation. In the next section we shall also meet the first-order term in the expansion of the scattering operator (1.14) relating these two dynamics,

$$S^{(1)}(s) = \Omega_-^{(1)}(s) - \Omega_+^{(1)}(s) = -\mathrm{i}\int_{-\infty}^{\infty} dt\, t\, \mathrm{e}^{\mathrm{i}H(s)t}\dot{H}(s)\mathrm{e}^{-\mathrm{i}H(s)t}\,. \tag{4.5}$$

The reason $\Omega_-^{(1)}(s)$, rather than $\Omega_+^{(1)}(s)$, appears in (4.2) is that the initial condition was set in the past of the current measurement.

(iv) All estimates in this section hold true uniformly in $s \in I$, $s_- \le 0$. Constants, however, may depend on a.

The two dynamics, U_ε and u_s, are compared by means of the Duhamel formula

$$U_\varepsilon(s',s) = u_s(s'-s) + \mathrm{i}\varepsilon^{-1}\int_{s'}^{s} ds_1 U_\varepsilon(s',s_1)(H(s_1)-H(s))u_s(s_1-s)\,. \tag{4.6}$$

Starting at epoch s, the Heisenberg dynamics of the currents carries them through the scatterer within a finite time, i.e., essentially still at the same epoch s. When applying (4.6) to $I_\pm(s,a)$, it is thus appropriate to linearize $H(s_1)-H(s)$ around s. The next lemma essentially says that when one calculates the current to first order in ε, the error is second order in ε.

LEMMA 4.2 *We have*

$$\varepsilon^{-1}\|[U_\varepsilon(s_-,s)-(u_s(s_--s)+X_\varepsilon(s_-,s))]I_\pm(s,a)\|_1\le C\varepsilon\,, \tag{4.7}$$

where

$$X_\varepsilon(s_-,s)=\mathrm{i}\varepsilon^{-1}\int_{s_-}^{s}ds_1(s_1-s)U_\varepsilon(s_-,s_1)\dot H(s)u_s(s_1-s)\,.$$

This, in turn, yields the following expression for the (rescaled) currents at epoch s:

$$\begin{aligned}
&\varepsilon^{-1}\,\mathrm{tr}\big(\rho(H_-)U_\varepsilon(s_-,s)I_\pm(s,a)U_\varepsilon(s,s_-)\big)\\
&\quad=\varepsilon^{-1}\,\mathrm{tr}\big(u_s(s-s_-)\rho(H_-)u_s(s_--s)I_\pm(s,a)\big)\\
&\qquad+\varepsilon^{-1}\,\mathrm{tr}\big(X_\varepsilon(s_-,s)^*\rho(H_-)u_s(s_--s)I_\pm(s,a)\big)\\
&\qquad+\varepsilon^{-1}\,\mathrm{tr}\big(u_s(s-s_-)\rho(H_-)X_\varepsilon(s_-,s)I_\pm(s,a)\big)\\
&\qquad+\varepsilon^{-1}\,\mathrm{tr}\big(\rho(H_-)X_\varepsilon(s_-,s)I_\pm(s,a)X_\varepsilon(s_-,s)^*\big)+\mathrm{O}(\varepsilon)\,.
\end{aligned}\tag{4.8}$$

PROOF: Using Duhamel's formula (4.6) and

$$H(s_1)-H(s)-(s_1-s)\dot H(s)=(H(s_1)-H(s)-(s_1-s)\dot H(s))F(A=0)\,,$$

$$\|H(s_1)-H(s)-(s_1-s)\dot H(s)\|\le C|s_1-s|^2\quad\text{(see (1.4))},$$

assumption (A1), and $\Pi_0=F(A=0)\Pi_0$, we are left with showing that

$$\varepsilon^{-2}\int_{s_-}^{s}ds_1\,|s_1-s|^2\cdot\|F(A=0)u_s(s_1-s)I_\pm(s,a)\|_1\le C\varepsilon\,. \tag{4.9}$$

We insert $1=F(A\le a+\alpha)+F(A>a+\alpha)$ to the left of the commutator in (1.11). By (3.3) and (3.8) the trace norm appearing under the integral is bounded as

$$\begin{aligned}
&\|F(A=0)u_s(s_1-s)I_\pm(s,a)\|_1\le\\
&\qquad C\|F(A=0)u_s(s_1-s)\chi(H(s))F(A\le a+\alpha)\|+C_N(1+\alpha)^{-N}\,,
\end{aligned}$$

where we also used (3.6). By (3.2) with $b=0$, the latter norm is estimated as

$$\begin{aligned}
&\|F(A=0)u_s(s_1-s)\chi(H(s))F(A\le a+\alpha)\|\le\\
&\qquad C\|F(A=0)F(A\le a+\alpha+\theta\varepsilon^{-1}(s_1-s))\|+C_N(1+\varepsilon^{-1}|s_1-s|)^{-N}\,.
\end{aligned}\tag{4.10}$$

Picking $\alpha=\frac{1}{2}\theta\varepsilon^{-1}(s-s_1)>0$, the first term vanishes for $s-s_1>2a\theta^{-1}\varepsilon$. Now equation (4.9) holds because the left-hand side is estimated by a constant times

$$\varepsilon^{-2}\int_0^\infty d\sigma\,\sigma^2(F(\sigma\le 2a\theta^{-1}\varepsilon)+(1+\varepsilon^{-1}\sigma)^{-N})\le C(\varepsilon a^3+\varepsilon)\,, \tag{4.11}$$

which proves the lemma. □

For what follows, we retain the following estimate from the above proof:

$$\left\| F(A=0)\mathrm{e}^{-\mathrm{i}H(s)t} I_\pm(s,a)\right\| \le F(|t| \le 2a\theta^{-1}) + C_N(1+|t|)^{-N}\,. \tag{4.12}$$

In particular, it proves the first remark after Proposition 4.1.

The last term in equation (4.8) is also $\mathrm{O}(\varepsilon)$, as shown by the next estimate.

LEMMA 4.3 *We have*

$$\left\| X_\varepsilon(s_-,s) I_\pm(s,a) X_\varepsilon(s_-,s)^*\right\|_1 \le C\varepsilon^2\,. \tag{4.13}$$

PROOF: As in the proof of the previous lemma, the norm in inequality (4.13) is bounded by

$$\begin{aligned} \varepsilon^{-2}\int_{s_-}^{s} ds_1\, ds_2 |s_1-s|\,|s_2-s| \\ \left\| F(A=0) u_s(s_1-s) I_\pm(s,a) u_s(s_2-s)^* F(A=0)\right\|_1\,. \end{aligned} \tag{4.14}$$

Using again (3.3) and (3.8), this last norm by itself is bounded by

$$\big(\|F(A=0)u_s(s_1-s)\chi(H(s))F(A\le a+\alpha)\| + C_N(1+\alpha)^{-N}\big)\cdot(s_1\to s_2)\,,$$

where $(s_1 \to s_2)$ is shorthand for the previous expression with s_1 replaced by s_2. We pick $\alpha = \frac{1}{2}\theta\varepsilon^{-1}\min(s-s_1, s-s_2) \ge 0$. Then the previous expression is estimated as

$$\left(F(\sigma_1 \le 2a\theta^{-1}\varepsilon) + \left(1+\frac{1}{2}\theta\varepsilon^{-1}\min(\sigma_1,\sigma_2)\right)^{-N}\right)\cdot(s_1\to s_2)\,,$$

where $\sigma_i = s - s_i$. Using

$$\int_0^\infty d\sigma_2\,\sigma_2\left(1+\frac{1}{2}\theta\varepsilon^{-1}\min(\sigma_1,\sigma_2)\right)^{-N} \le C\big(\sigma_1^2+\varepsilon^2\big)\,,$$

$$\int_0^\infty d\sigma_1\, d\sigma_2\,\sigma_1\sigma_2\left(1+\frac{1}{2}\theta\varepsilon^{-1}\min(\sigma_1,\sigma_2)\right)^{-N} \le C\varepsilon^4\,,$$

the claimed bound is established for (4.14). □

We now turn to the second and third terms in equation (4.8), which will account for the current in the adiabatic limit.

LEMMA 4.4

$$\begin{aligned} \lim_{\varepsilon\to 0}\Big\| (U_\varepsilon(s_-,s_1) - u_s(s_--s_1)) \\ \cdot u_s(s_1-s)\rho(H(s))\chi(H(s))(\pm A - a + \mathrm{i})^{-2}\Big\|_1 = 0\,, \end{aligned} \tag{4.15}$$

uniformly in $s_1 \in [s_-, s]$.

PROOF: We first consider the case where ρ is smooth. Because

$$T = \chi(H(s))(\pm A - a + \mathrm{i})^{-2} \in \mathcal{J}_1$$

by (A.16) and $\text{s-lim}_{\alpha\to\infty} F(A > \alpha) = 0$, we have $\lim_{\alpha\to\infty} \|F(A > \alpha)T\|_1 = 0$. By approximation we may thus prove

$$\lim_{\varepsilon\to 0} \left\|(U_\varepsilon(s_-, s_1) - u_s(s_- - s_1))u_s(s_1 - s)\rho(H(s))\tilde{\chi}(H(s))F(A \le \alpha)\right\| = 0\,,$$

where $\tilde{\chi} \in C_0^\infty(0,\infty)$ with $\tilde{\chi}\chi = \chi$. To estimate this operator norm we use (4.6) together with

$$\|H(s_2) - H(s)\| \le C|s_2 - s| \tag{4.16}$$

to obtain the bound

$$\varepsilon^{-1}\int_{s_-}^{s_1} ds_2 |s_2 - s| \|F(A = 0)u_s(s_2 - s)\rho(H(s))\tilde{\chi}(H(s))F(A \le \alpha)\| \\ \le C\varepsilon(1+\alpha^2)\,,$$

where we used that the norm of the integrand is bounded by

$$F\big(s - s_2 \le \varepsilon\theta^{-1}\alpha\big) + C_N\big(1 + \varepsilon^{-1}|s_2 - s|\big)^{-N}$$

(see the argument in connection with (4.10)). The general case, where ρ is of bounded variation, is also dealt with by approximating $\rho(H) = \text{s-lim}_{n\to\infty} \rho_n(H)$ with ρ_n smooth. In fact, we can pick n so that $\|(\rho_n(H) - \rho(H))T\|_1$ is arbitrarily small (uniformly in s). □

PROOF OF PROPOSITION 4.1: As mentioned in the introduction,

$$U_\varepsilon(s, s_-)\rho(H_-)U_\varepsilon(s_-, s)$$

is independent of $s_- \le 0$. We may thus evaluate the right-hand side of (4.8) in the limit $s_- \to \infty$. By estimate (3.15) and its adjoint, this amounts to replacing $\rho(H_-)$ by $\rho(H(s))$, i.e.,

$$\begin{aligned} &\varepsilon^{-1}\operatorname{tr}(\rho(H_-)U_\varepsilon(s_-, s)I_\pm(s,a)U_\varepsilon(s, s_-)) \\ &\quad = \varepsilon^{-1}\operatorname{tr}(\rho(H(s))I_\pm(s,a)) \\ &\qquad + \varepsilon^{-1}\lim_{s_-\to-\infty}\operatorname{tr}\big(X_\varepsilon(s_-, s)^* u_s(s_- - s)\rho(H(s))I_\pm(s,a)\big) \\ &\qquad + \varepsilon^{-1}\lim_{s_-\to-\infty}\operatorname{tr}\big(u_s(s - s_-)X_\varepsilon(s_-, s)I_\pm(s,a)\rho(H(s))\big) + \mathrm{O}(\varepsilon)\,, \end{aligned} \tag{4.17}$$

where we also used $[u_s(s - s_-), \rho(H(s))] = 0$ and (4.13). The first term on the right-hand side is just the equilibrium value of the current subtracted on the left-hand side of equation (4.2). Because we are not going to show that the limits in (4.17) exist, they are just to be understood as sets of limit points. We next claim that

$$\lim_{\varepsilon\to 0}\varepsilon^{-1}\lim_{s_-\to\infty}\operatorname{tr}\big((X_\varepsilon(s_-, s)^* u_s(s_- - s) - \varepsilon\Omega_-^{(1)}(s))\rho(H(s))I_\pm(s,a)\big) \to 0\,. \tag{4.18}$$

By taking the complex conjugate, this implies

$$\lim_{\varepsilon\to 0}\varepsilon^{-1}\lim_{s_-\to\infty}\operatorname{tr}\bigl(I_\pm(s,a)\rho(H(s))(u_s(s-s_-)X_\varepsilon(s_-,s)+\varepsilon\Omega_-^{(1)}(s))\bigr)\to 0\,,$$

where we used $\Omega_-^{(1)}(s)^*=-\Omega_-^{(1)}(s)$. Used together in (4.17), they prove (4.2).

We next note that, by a change of variables,

$$\varepsilon\Omega_-^{(1)}(s)=-\mathrm{i}\varepsilon^{-1}\int_{-\infty}^{s}ds_1(s_1-s)u_s(s-s_1)\dot H(s)u_s(s_1-s)\,.$$

As noted before, the integral is convergent in the trace class norm upon multiplication on either side by $I_\pm(s,a)$. For the purpose of proving (4.18), we may thus assume it to have s_- as the lower limit of integration. Then the trace there, including the factor ε^{-1} in front, equals

$$-\mathrm{i}\varepsilon^{-2}\int_{s_-}^{s}ds_1(s_1-s)\times$$
$$\operatorname{tr}\bigl(u_s(s-s_1)\dot H(s)(U_\varepsilon(s_1,s_-)u_s(s_--s)-u_s(s_1-s))\rho(H(s))I_\pm(s,a)\bigr)\,.$$

We use

$$U_\varepsilon(s_1,s_-)u_s(s_--s)-u_s(s_1-s)=$$
$$U_\varepsilon(s_1,s_-)(u_s(s_--s_1)-U_\varepsilon(s_-,s_1))u_s(s_1-s)$$

and turn $u_s(s-s_1)\dot H(s)$ around the trace, so that the previous expression is estimated as

$$\varepsilon^{-2}\int_{s_-}^{s}ds_1|s_1-s|$$
$$\cdot\left\|(U_\varepsilon(s_-,s_1)-u_s(s_--s_1))u_s(s_1-s)\rho(H(s))\chi(H(s))(\pm A-a+\mathrm{i})^{-2}\right\|_1$$
$$\cdot\left\|(\pm A-a+\mathrm{i})^2[H_b(s),f(\pm A-a)]\chi(H(s))u_s(s-s_1)F(A=0)\right\|\,.$$

The first factor tends to zero uniformly as $\varepsilon\to 0$ by (4.15), so we are left to show

$$\varepsilon^{-2}\int_{s_-}^{s}ds_1|s_1-s|\cdot \tag{4.19}$$
$$\left\|F(A=0)u_s(s_1-s)\chi(H(s))[H_b(s),f(\pm A-a)](\pm A-a+\mathrm{i})^2\right\|\le C\,.$$

We insert $1=F(A\le a+\alpha)+F(A>a+\alpha)$ to the left of the commutator. By (3.6), (3.8), and the remark following them, we obtain the bound

$$\varepsilon^{-2}\int_{s_-}^{s}ds_1|s_1-s|\cdot$$
$$\bigl(\|F(A=0)u_s(s_1-s)\chi(H(s))F(A\le a+\alpha)\|+C_N(1+\alpha)^{-N}\bigr)\,,$$

where we take $\alpha=\frac{1}{2}\theta\varepsilon^{-1}(s-s_1)>0$ as in (4.10). The resulting bound differs from (4.11) by having σ instead of σ^2. Hence we have the bound (4.19). □

5 The Scattering Limit

In the previous section we saw that the currents can be computed from frozen data in the adiabatic limit. These data were not directly related to the frozen scattering data and involved objects like $H(s)$ and $\Omega_-^{(1)}(s)$. In this section we show that in the limit that the ammeter is far from the pump, $a \to \infty$, then all we need to know is the frozen, scattering operator S and the initial state ρ.

First we show that in the large a limit, the incoming and outgoing currents have no scattering in the past and future, respectively. As usual, all statements are uniform in $s \in I$.

LEMMA 5.1 *We have*

$$\lim_{a\to\infty} \|\Omega_-^{(1)}(s) I_-(s,a)\|_1 = 0\,,$$
$$\lim_{a\to\infty} \|(\Omega_-^{(1)}(s) - S^{(1)}(s)) I_+(s,a)\|_1 = 0\,.$$

We recall that $S^{(1)}$ was defined in (4.5). These facts will yield a first expression for the scattering limit of the current, equation (4.4).

LEMMA 5.2 *We have*

$$\lim_{a\to\infty} \operatorname{tr}\big([\Omega_-^{(1)}(s), \rho(H(s))](I_+(s,a) + I_-(s,a))\big) = \operatorname{tr}\big([S^{(1)}(s), \rho(H(s))] I_+(s,a)\big)\,, \tag{5.1}$$

where a on the right-hand side is arbitrary.

We then express the latter result in terms of "frozen" scattering data, such as the scattering operator $S(s)$, defined in (1.9). Notice that it acts on the asymptotic Hilbert space $L^2(\mathbb{R}_+, \mathbb{C}^n)$ of the channels, rather than on $\mathcal{H}$. Further distinguished operators acting there are the Neumann Hamiltonian H_0, introduced in the introduction, and the generator of dilations,

$$A_0 = \frac{1}{2\mathrm{i}}\left(\frac{d}{dx}x + x\frac{d}{dx}\right),$$

which may be regarded as a model for (1.6). The trace (5.1) can then finally be computed exactly.

PROPOSITION 5.3 *Suppose, in addition to the hypotheses of Theorem* 1.1*, that ρ is smooth. Then*

$$\operatorname{tr}\big([S^{(1)}(s), \rho(H(s))] I_+(s,a)\big)$$
$$= -\mathrm{i}\operatorname{tr}\big(\dot S(s) S(s)^* \rho'(H_0)\Pi_j \mathrm{i}[H_0, f(A_0 - a)]\big) \tag{5.2}$$
$$= -\frac{\mathrm{i}}{2\pi}\int_0^\infty d\rho(E)\left(\frac{dS}{ds}S^*\right)_{jj}\,, \tag{5.3}$$

where the scattering operator $S(s)$ is defined in equation (1.9) *and* $A_{0j} = A_0\Pi_j$.

For ρ not smooth, an approximation argument will complete the task.

PROOF OF LEMMA 5.1: Both claims of this proposition are consequences of the stronger bound

$$\left\|\Omega_{\pm}^{(1)}(s)I_{\pm}(s,a)\right\|_1 \le C_N a^{-(N-2)}$$

for large enough N. Let us prove this bound for a case of Ω_-; the proof for Ω_+ follows the same lines.

It is clear from equation (4.3) that we may establish that bound for

$$\int_{-\infty}^{0} dt|t| \cdot \|F(A=0)\mathrm{e}^{-\mathrm{i}H(s)t} I_-(s,a)\|_1 .$$

The norm under this integral also appeared under the integral (4.9). We estimate it similarly by means of (3.3) and (3.8), except that we insert $F(A \le -a+\alpha)$ (and the complementary projection) instead of $F(A \le a+\alpha)$. By (3.2) we get

$$\begin{aligned}\|F(A=0)\mathrm{e}^{-\mathrm{i}H(s)t} I_-(s,a)\|_1 \le C\|F(A=0)F(A \le -a+\alpha-b+\theta t)\| \\ + C_N(|b|+|t|)^{-N} + C_N\alpha^{-N} .\end{aligned}$$

Choosing $b=-a/2$ and $\alpha=(a/2-\theta t)/2>0$, we see that the first term vanishes, and we obtain the desired bound since

$$\int_{-\infty}^{0} dt\,|t|\left(\frac{a}{2}+\theta|t|\right)^{-N} \le C_N a^{-(N-2)} .$$

□

The main ingredients in the proof of Proposition 5.3 and, to a minor extent, of Lemma 5.2, are the relations equations (1.15) and (1.16). Formally, equation (1.15) follows for $\rho(\lambda)=\mathrm{e}^{\mathrm{i}\lambda t}$, $t\in\mathbb{R}$, by a change of variables in (1.14) and hence for general functions ρ. For our purposes we shall need a somewhat more precise statement, given by the first part of the following lemma (cf. the first remark after Proposition 4.1).

LEMMA 5.4

(i) *Equation* (1.16) *and, for* ρ *smooth, equation* (1.15) *hold true if multiplied on either side by* $I_+(s,a)$.

(ii) *The wave operators* $\Omega_{\pm}(s',s)=\text{s-lim}_{T\to\pm\infty}\mathrm{e}^{\mathrm{i}H(s')T}\mathrm{e}^{-\mathrm{i}H(s)T}P_{\mathrm{ac}}(H(s))$ *for the pair* $(H(s'),H(s))$ *satisfy the intertwining property*

$$f(H(s'))\Omega_{\pm}(s',s)=\Omega_{\pm}(s',s)f(H(s)) \tag{5.4}$$

for any (*Borel*) *function* f.

(iii) *The scattering operators for the pairs* $(H(s),H(s_i))$, $i=1,2$, *are related by*

$$S(s,s_2)=\Omega_+(s_2,s_1)S(s,s_1)\Omega_-(s_2,s_1)^* . \tag{5.5}$$

PROOF: Parts (ii) and (iii) are standard [5, 20]. The wave operators exist and are complete under our assumptions. The chain rule for wave operators,

$$\Omega_\pm(s, s_1) = \Omega_\pm(s, s_2)\Omega_\pm(s_2, s_1)\,,$$

and $S(s, s_i) = \Omega_+(s, s_i)^*\Omega_-(s, s_i)$ imply

$$S(s, s_1) = \Omega_+(s_2, s_1)^* S(s, s_2)\Omega_-(s_2, s_1)\,.$$

From this (5.5) follows by the completeness of scattering,

$$\Omega_\pm(s_2, s_1)^*\Omega_\pm(s_2, s_1) = P_{\mathrm{ac}}(H(s_2))\,.$$

We begin the proof of part (i) by claiming that

$$\|(\Omega_+(s', s) - 1)\chi(H(s))\| \le C|s' - s|\,, \tag{5.6}$$

where $\chi \in C_0^\infty(0, \infty)$. Indeed, let $\tilde\chi \in C_0^\infty(0, \infty)$ with $\tilde\chi\chi = \chi$. Then, by (5.4),

$$\begin{aligned}\|(\Omega_+ - 1)\chi(H(s))\| \le{}& \|\tilde\chi(H(s'))(\Omega_+ - 1)\chi(H(s))\| \\ &+ \|\tilde\chi(H(s'))\chi(H(s)) - \chi(H(s))\|\,.\end{aligned}$$

The second term is bounded by $\|\tilde\chi(H(s')) - \tilde\chi(H(s))\|$ and fits the bound (5.6) by (A.5). For the first term we use the fundamental theorem of calculus:

$$\begin{aligned}&\tilde\chi(H(s'))(\Omega_+(s', s) - 1)\chi(H(s)) = \\ &\qquad \operatorname*{s-lim}_{T\to\infty} \mathrm{i}\int_0^T dt\, \tilde\chi(H(s'))\mathrm{e}^{\mathrm{i}H(s')t} V \mathrm{e}^{-\mathrm{i}H(s)t}\chi(H(s))\,,\end{aligned} \tag{5.7}$$

where $V = H(s') - H(s)$. We write $V = \langle A\rangle^{-r} V \langle A\rangle^{-r}$ and use (4.16) for V, as well as the $H(s)$-smoothness of $\langle A\rangle^{-r}\chi(H(s))$ for $r > \frac{1}{2}$ (and similarly for s'); see item (ii) in Section 2. An application of the Cauchy-Schwarz inequality on matrix elements of (5.7) yields (5.6).

We can now prove the statement about equation (1.16), whose right-hand side we denote by T. Then $TI_+(s, a)$ is a convergent integral by (4.12). Moreover, $T\mathrm{e}^{-\mathrm{i}H(s)t} I_+(s, a) = \mathrm{e}^{-\mathrm{i}H(s)t} T I_+(s, a)$, whence

$$T\tilde\chi(H(s))I_+(s, a) = \tilde\chi(H(s))TI_+(s, a)$$

for $\tilde\chi \in C_0^\infty(0, \infty)$. Since $\tilde\chi(H(s))I_+(s, a) = I_+(s, a)$ for $\tilde\chi\chi = \chi$ and χ as in (1.11), we may thus prove

$$\begin{aligned}&\tilde\chi(H(s))\partial_{s'} S(s', s)_{s'=s} I_+(s, a) = \\ &\qquad -\mathrm{i}\tilde\chi(H(s))\int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}H(s)t}\dot H(s)\mathrm{e}^{-\mathrm{i}H(s)t} I_+(s, a)\,.\end{aligned} \tag{5.8}$$

We write $S-1=\Omega_+^*(\Omega_- - \Omega_+)$, so that

$$\begin{aligned}
&\tilde\chi(H(s))(S(s',s)-1)I_+(s,a)\\
&\quad= -\mathrm{i}\tilde\chi(H(s))\Omega_+^*\int_{-\infty}^{\infty}dt\,\mathrm{e}^{\mathrm{i}H(s')t}V\mathrm{e}^{-\mathrm{i}H(s)t}I_+(s,a)\\
&\quad= -\mathrm{i}\int_{-\infty}^{\infty}dt\,\mathrm{e}^{\mathrm{i}H(s)t}\tilde\chi(H(s))(\Omega_+^*-1)V\mathrm{e}^{-\mathrm{i}H(s)t}I_+(s,a)\\
&\qquad -\mathrm{i}\tilde\chi(H(s))\int_{-\infty}^{\infty}dt\,\mathrm{e}^{\mathrm{i}H(s)t}V\mathrm{e}^{-\mathrm{i}H(s)t}I_+(s,a)\,.
\end{aligned}$$

The first integral is estimated as $C(a)|s'-s|^2$ due to equations (5.6), (4.16), and (4.12). In the second one, the contribution coming from the remainder in $V=\dot H(s)(s'-s)+O((s'-s)^2)$ is estimated the same way. This implies (5.8).

As for equation (1.15) in the case $\rho(\lambda)=\mathrm{e}^{\mathrm{i}\lambda t}$, the change of variables mentioned before is legitimate, because the integrals are convergent once multiplied by $I_+(s,a)$ due to (4.12). The result extends to $\rho(H(s))$ with $\rho\in C_0^\infty(\mathbb{R})$ or $\rho'\in C_0^\infty(\mathbb{R})$, which amounts to the same since $H(s)$ is bounded below. $\square$

PROOF OF LEMMA 5.2: By Lemma 5.1 the left-hand side of (5.1) equals

$$\lim_{a\to\infty}\mathrm{tr}\big([S^{(1)}(s),\rho(H(s))]I_+(s,a)\big)\,,$$

provided this limit exists. It does, since the expression is independent of a. For ρ smooth, this follows from Lemma 5.4. Indeed, the right-hand side of (1.15) commutes with $H(s)$, so that the independence is seen as in (2.3). For general ρ, the conclusion follows by approximation by a sequence $\{\rho_n\}$ of smooth functions such that s-lim $\rho_n(H(s))=\rho(H(s))$. The traces converge by (3.19). $\square$

PROOF OF PROPOSITION 5.3: For the sake of precision we recall that the scattering operator $S(s)=\Omega_+(s)^*\Omega_-(s)$ depends on wave operators defined in a setting of two Hilbert spaces: $\Omega_\pm(s)=\text{s-lim}_{T\to\pm\infty}\,\mathrm{e}^{\mathrm{i}H(s)T}J\mathrm{e}^{-\mathrm{i}H_0T}$, where

$$J: L^2(\mathbb{R}_+,\mathbb{C}^n)\to\mathcal{H}$$

is the embedding given by (1.2). We may also replace J by a smooth function $\tilde J$ on $\mathbb{R}$, which is 0 near $x=0$, and 1 near $x=\infty$. This is without effect on $\Omega_\pm(s)$, since $\text{s-lim}_{T\to\pm\infty}(J-\tilde J)\mathrm{e}^{-\mathrm{i}H_0T}=0$. In particular, we may pick $\tilde J$ so that $\tilde J=1$ on supp v; see (1.6). In the present context, (5.5) reads $S(s',s)=\Omega_+(s)S(s')\Omega_-(s)^*$ and implies

$$\partial_{s'}S(s',s)_{s'=s}=\Omega_+(s)\dot S(s)\Omega_-(s)^*\,,$$

where the differentiability is granted after multiplication by $I_+(s,a)$.

We now prove equation (5.2) with $\Pi_j \mathrm{i}[H_0, f(A-a)] = \mathrm{i}[H_0, f(A_j - a)]$ instead of $\Pi_j \mathrm{i}[H_0, f(A_0 - a)]$. Its left-hand side equals, by Lemma 5.4,

$$\begin{aligned}
&\operatorname{tr}\big(\Omega_+(s)\dot{S}(s)\Omega_-(s)^*\rho'(H(s))\chi(H(s))I_+(a)\chi(H(s))\big)\\
&\quad= \operatorname{tr}\big(\dot{S}(s)S(s)^*\rho'(H_0)\chi(H_0)I_+(a)\chi(H_0)\big)\\
&\qquad+ \operatorname{tr}\big(\dot{S}(s)\Omega_-(s)^*\rho'(H(s))\chi(H(s))[I_+(a),\Omega_+(s)]\chi(H_0)\big)\,.
\end{aligned}$$

Here $I_+(a)$ is defined in equation (1.7). We turned $\Omega_+(s)$ around the trace, which thereby moved from $\mathcal{H}$ to $L^2(\mathbb{R}_+, \mathbb{C}^n)$. The first term corresponds to the claim, since $\chi\rho'\chi = \rho'$. It is again independent of a. The second term will thus vanish as soon as it does in limit $a \to \infty$. The commutator there is $[I_+(a), \Omega_+(s)] = [I_+(a), \Omega_+(s) - \tilde{J}]$ by the above choice $\tilde{J}$. We are thus led to show that

$$\lim_{a\to\infty} \big\|\chi(H(s))(\Omega_+(s) - \tilde{J})\chi(H_0)I_+(a)\big\|_1 = 0\,,$$

and also with $\Omega_+(s)$ replaced by $\Omega_+(s)^*$, and $\chi(H_0)$ and $\chi(H(s))$ switched. Using the integral representation for $\Omega_+(s) - \tilde{J}$, the estimate reduces to

$$\begin{aligned}
&\int_0^\infty dt\,\big\|\chi(H(s)[H_0,\tilde{J}]\chi(H_0)\mathrm{e}^{-\mathrm{i}H_0 t}I_+(a)\big\|_1 \le\\
&\qquad\qquad C\int_0^\infty dt\,\big\|F(A=0)\chi(H_0)\mathrm{e}^{-\mathrm{i}H_0 t}I_+(a)\big\|_1 \to 0\,,\quad a\to\infty\,,
\end{aligned}$$

(and with H_0 and $H(s)$ interchanged), which holds true by the estimates in the proof of Lemma 5.1.

We next replace A by A_0 on the right-hand side of (5.2). Since both traces are independent of a, we may, in each of them, replace f by a smeared switch function $\tilde{f}'$, such that $\tilde{f} \in H^2(d)$ with $d > 2$ (see the appendix for notation). Since $(\tilde{f}(A_j) - \tilde{f}(A_{0j}))\rho'(H_0) \in \mathcal{J}_1$ by (A.12), the difference is seen to vanish by cyclicity.

Finally, to prove (5.3), we may keep f replaced by $\tilde{f}$ as before. It follows from equations (A.2) and (A.10) that

$$\begin{aligned}
&\operatorname{tr}\big(\dot{S}(s)S(s)^*\rho'(H_0)\Pi_j[H_0,\tilde{f}(A_0 - a)]\big)\\
&\quad= \operatorname{tr}\big(\dot{S}(s)S(s)^*\rho'(H_0)\Pi_j(\tilde{f}(A_0 - a - 2\mathrm{i}) - \tilde{f}(A_0 - a))H_0\big)\\
&\quad= \frac{1}{2\pi}\int_0^\infty \frac{dE}{2E}\rho'(E)E\left(\frac{dS}{ds}S^*\right)_{jj}\cdot\int_{-\infty}^\infty d\lambda(\tilde{f}(\lambda - a - 2\mathrm{i}) - \tilde{f}(\lambda - a))\,.
\end{aligned}$$

To compute the last integral, note that $\int_{-\infty}^\infty d\lambda(\tilde{f}(\lambda - c) - \tilde{f}(\lambda)) = -c$ for any $c \in \mathbb{R}$ that extends by analyticity to $|\operatorname{Im} c| < d$. Hence the result. □

PROOF OF THEOREM 1.1: We have shown that

$$\operatorname{tr}\big([S^{(1)}(s), \rho(H(s))]I_+(s,a)\big) = -\frac{\mathrm{i}}{2\pi}\int_0^\infty d\rho(E)\left(\frac{dS}{ds}S^*\right)_{jj} \tag{5.9}$$

holds true if ρ is smooth. If ρ is of bounded variation, it can be approximated by a sequence $\rho_n \in C_0^\infty(\mathbb{R})$ with $\rho_n(\lambda) \to \rho(\lambda)$ pointwise and uniformly bounded total variation $\sup_n V(\rho_n) < \infty$. Then

$$\operatorname*{s-lim}_n \rho_n(H(s)) = \rho(H(s))$$

and $d\rho_n(\lambda) \to d\rho(\lambda)$ in the sense of weak-star convergence. Hence (5.9) is inherited by the limit. The proof is completed by equations (4.4) and (5.1). □

Appendix: Trace Class Properties of $g(H)f(A)$

Here we discuss different properties of the operator product $g(H(s))f(A)$. We first prove that operators of the form $g(H_0)f(A_0)$ are Hilbert-Schmidt under suitable conditions on the functions g and f. For operators of this type one can essentially write down the integral kernel and use it to compute the Hilbert-Schmidt norm. Heuristically the trace of an operator is the integral over phase space of the symbol (divided by 2π). Since

$$\frac{1}{2\pi}\int dx\,dp = \frac{1}{2\pi}\int \frac{dE}{2E}da$$

under the map $(x, p) \mapsto (E = p^2, a = px)$, we introduce the norms

$$\|f\|^2 = \int_{-\infty}^{\infty} da\,|f(a)|^2\,, \quad |||g|||^2 = \int_0^\infty \frac{dE}{2E}|g(E)|^2$$

for functions f on the real line and g on the half-line, respectively. The Fourier transform is $\hat{f}(t) = (2\pi)^{-1}\int e^{-i\lambda t} f(\lambda)d\lambda$.

PROPOSITION A.1 *We have*

$$\|g(H_0)f(A_0)\|_2 = (2\pi)^{-1/2}|||g|||\cdot\|f\|\,. \tag{A.1}$$

If g and $\hat{f}$ are continuous and the operator $g(H_0)f(A_0)$ is trace class, then

$$\operatorname{tr}(g(H_0)f(A_0)) = \frac{1}{2\pi}\int_0^\infty \frac{dE}{2E}g(E)\cdot\int_{-\infty}^{\infty} da\,f(a)\,. \tag{A.2}$$

PROOF: The space $L^2(\mathbb{R}_+)$ can be identified with the even functions in $L^2(\mathbb{R})$ by means of the map $(J\varphi)(x) = \varphi(|x|)$ with $\|J\varphi\|^2 = 2\|\varphi\|^2$. Consider the operator $g(p^2)f(A_0)$ on $L^2(\mathbb{R})$. Since it preserves parity and p^2 reduces to H_0 on the (so identified) subspace of even functions (with projection P_+), we have

$$\begin{aligned}\|g(H_0)f(A_0)\|_2^2 &= \operatorname{tr}_{L^2(\mathbb{R}_+)}\big(\bar{g}(H_0)|f|^2(A_0)g(H_0)\big)\\ &= \frac{1}{2}\operatorname{tr}_{L^2(\mathbb{R})}\big(P_+\bar{g}(p^2)|f|^2(A_0)g(p^2)P_+\big)\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\,\mathrm{tr}_{L^2(\mathbb{R})}\big(U^* P_+ \bar{g}(p^2)|f|^2(A_0) g(p^2) P_+ U\big)\\
&= \frac{1}{2}\,\mathrm{tr}_{L^2(\mathbb{R})}\big(P_+ \bar{g}(x^2)|f|^2(-A_0) g(x^2) P_+\big)\\
&= \mathrm{tr}_{L^2(\mathbb{R}_+)}\big(\bar{g}(x^2)|f|^2(-A_0) g(x^2)\big)\,, \qquad \text{(A.3)}
\end{aligned}
$$

where $(U\psi)(k) = (2\pi)^{1/2}\hat{\psi}(k)$ is the Fourier transform: $[U, P_+] = 0$, $P_+ = (1+U^2)/2$, $pU = -Ux$, and $A_0 U = -A_0 U$. Using the Mellin transform $M : L^2(\mathbb{R}_+) \to L^2(\mathbb{R})$,

$$
(M\varphi)(a) = (2\pi)^{-1/2}\int_0^\infty \frac{dx}{x^{1/2}} x^{-\mathrm{i}a}\varphi(x)\,,
$$

which diagonalizes $A_0 = M^* a M$, one obtains that $h(a)$ has integral kernel

$$
h(A)(x, y) = (2\pi)^{-1}(xy)^{-\frac{1}{2}}\hat{h}\left(\log\frac{y}{x}\right) \qquad \text{(A.4)}
$$

for $h \in L^1(\mathbb{R})$. Since the kernel is continuous in $x, y > 0$, we can write for (A.3) (cf. [22, theorem 3.9])

$$
(2\pi)^{-1}\int_0^\infty \frac{dx}{x}|g(x^2)|^2 \int_{-\infty}^\infty da\,|f|^2(-a)\,.
$$

By means of the change of variable $x^2 = E$, this is the square of the right-hand side of (A.1).

We find $\mathrm{tr}(g(H_0)f(A_0)) = \mathrm{tr}(g(x^2)f(-A_0))$ by using the Fourier transform as in (A.3). The integral kernel of the latter operator is obtained from (A.4), and the trace is the integral over its diagonal due to [22, theorem 3.9]. □

In the rest of this appendix, we shall give an example of the trace class operator involving A_0 and H_0 and use it to establish $g(H(s))f(A) \in \mathcal{J}_1$ for a large enough class of operators.

LEMMA A.2 *Let $g \in C_0^\infty(\mathbb{R})$; then*

$$
\|g(H(s)) - g(H(s'))\|_1 \le C|s - s'|\,, \qquad \text{(A.5)}
$$

$$
g(H(s)) - Jg(H_0)J^* \in \mathcal{J}_1\,, \qquad \text{(A.6)}
$$

where $J : L^2(\mathbb{R}_+, \mathbb{C}^n) \to \mathcal{H}$ is the embedding given by (1.2).

PROOF: We first prove (A.5) for $g(\lambda) = (\lambda+\mathrm{i})^{-2m}$, where m is as in assumption (A2). Setting $R(s) = (H(s)+\mathrm{i})^{-1}$ we have by (1.4) and the resolvent identity

$$
\begin{aligned}
R(s)^{2m} - R(s')^{2m} &= \sum_{k=1}^{2m} R(s)^{2m-k}(R(s) - R(s'))R(s')^{k-1}\\
&= \sum_{k=1}^{2m} R(s)^{2m-k+1}\Pi_0(H(s') - H(s))\Pi_0 R(s')^k\,.
\end{aligned}
$$

The desired bound now follows from (A1) by using (A2) either for s or s'. For general $g \in C_0^\infty(\mathbb{R})$, as well as for the rest of this proof, we use the Helffer-Sjöstrand representation,

$$g(H) = \frac{1}{\pi} \int_{\mathbb{R}^2} (H - z)^{-1} \partial_{\bar{z}} \tilde{g}(z) dx\, dy\,, \tag{A.7}$$

where $\partial_{\bar{z}} = (\partial_x + \mathrm{i}\partial_y)/2$, and $\tilde{g}$ is an almost-analytic extension of g with $\tilde{g}(z)$ vanishing to a high power near the real axis. Before doing that, we set $G(\lambda) = g(\lambda)(\lambda + \mathrm{i})^{2m}$, so that the first term in

$$\begin{aligned} g(H(s)) - g(H(s')) = (R(s)^{2m} - R(s')^{2m}) G(H(s')) \\ + R(s)^{2m}(G(H(s)) - G(H(s')) \end{aligned}$$

is taken care of. For the second, we apply (A.7) to G and are led to the estimate

$$\begin{aligned} &\left\| R(s)^{2m}[(H(s) - z)^{-1} - (H(s') - z)^{-1}] \right\|_1 \\ &\leq \left\| (H(s) - z)^{-1} \right\| \left\| R(s)^{2m} \Pi_0 \right\|_1 \left\| H(s') - H(s) \right\| \left\| (H(s') - z)^{-1} \right\| \\ &\leq C |\mathrm{Im}\, z|^{-2} |s - s'|\,, \end{aligned}$$

which completes the proof of (A.5).

Before proving (A.6) we claim that

$$g(H)h \in \mathcal{J}_1\,, \tag{A.8}$$

where h acts as multiplication by $h \in C_0^\infty[0, \infty)$ on $L^2(\mathbb{R}_+, \mathbb{C}^n)$ and by $h(0)$ on $\mathcal{H}_0$. Since $g(H)\Pi_0 \in \mathcal{J}_1$, it will be enough to show $(1 - \Pi_0)g(H)(1 - \Pi_0)h \in \mathcal{J}_1$ or actually just $\| J(H - z)^{-1} J^* h(x) \|_1 \leq C |\mathrm{Im}\, z|^{-1}$. Since the kernel of $(H - z)^{-1}$ is decaying exponentially [9], matters are further reduced to

$$\left\| J_L (H - z)^{-1} J_L^* \right\|_1 \leq C |\mathrm{Im}\, z|^{-1}$$

as an operator on $L^2([0, L], \mathbb{C}^n)$, where J_L is the corresponding embedding operator into $\mathcal{H}$. The initial piece $[0, L]$ has to be taken large enough, so that $\mathrm{supp}\, h \subset [0, L)$. Now let B be the quadratic form of the bi-Laplacian,

$$B(\varphi, \psi) = \int_0^L \bar{\varphi}''(x) \psi''(x) dx\,, \tag{A.9}$$

with domain given by the Sobolev space $W^2(0, L)$. We maintain that

$$\left\| (1 + B)^{1/2} J_L (H - z)^{-1} J_L^* \right\| \leq C |\mathrm{Im}\, z|^{-1}\,, \quad (1 + B)^{-1/2} \in \mathcal{J}_1\,,$$

which implies the claim. The first statement follows by (A3) and (A.9) from

$$J_L (H - \bar{z})^{-1} J_L^* B J_L (H - z)^{-1} J_L^* = T^* T\,,$$

with $T = 1 + z J_L (H - z)^{-1} J_L^*$. The second statement can be seen by computing the eigenvalues k^4 of the operator B associated to (A.9). The latter is given as $B = d^4/dx^4$ with boundary conditions $\varphi'' = \varphi''' = 0$ at $x = 0, L$. From this one computes the eigenvalues as the zeros of $1 - \cosh kL \cos kL$.

To prove (A.6), we make use of a smooth embedding $\tilde{J}$ as in the proof of Proposition 5.3. Since $(J - \tilde{J})g(H_0) \in \mathcal{J}_1$ (see [20, theorem XI.20]) we will prove the trace class property for

$$g(H) - \tilde{J}g(H_0)\tilde{J}^* = g(H)(1 - \tilde{J}\tilde{J}^*) + (g(H)\tilde{J} - \tilde{J}g(H_0))\tilde{J}^* .$$

The first term is trace class by (A.8). For the second term, equation (A.7) and the resolvent identity reduce matters to

$$\begin{aligned}\left\|(H-z)^{-1}[\tilde{J}, H](H_0 - z)^{-1}\tilde{J}^*\right\|_1 &\le \left\|(H-z)^{-1}[\tilde{J}, H]\right\| \left\|h(x)(H_0 - z)^{-1}\right\|_1 \\ &\le C|\mathrm{Im}\, z|^{-2} ,\end{aligned}$$

where $h \in C_0^\infty(\mathbb{R})$ with $h\tilde{J}' = \tilde{J}'$. □

The Hardy class $H^2(d)$ consists of all functions f that are analytic in the strip $\{z : |\mathrm{Im}\, z| < d\}$ and satisfy

$$\sup_{-d<y<d} \int_{-\infty}^{\infty} |f(x + \mathrm{i}y)|^2\, dx < \infty .$$

We recall that $\sup_{0<y<d} \|\mathrm{e}^{y|k|}\hat{f}(k)\|_2 < \infty$ for $f \in H^2(d)$.

PROPOSITION A.3 (The Pull-through Formula) *For any $f \in H^2(d)$ with $d > 2$,*

$$H_0 f(A_0) = f(A_0 - 2\mathrm{i})H_0 . \tag{A.10}$$

PROOF: We first prove the statement for $f(x) = \mathrm{e}^{-\mathrm{i}tx}$. Under conjugation with the dilation operator, $(\mathrm{e}^{-\mathrm{i}tA_0}\psi)(x) = \mathrm{e}^{-t/2}\psi(e^{-t}x)$, the Neumann Laplacian becomes

$$\mathrm{e}^{\mathrm{i}tA_0} H_0 \mathrm{e}^{-\mathrm{i}tA_0} = e^{-2t} H_0 ; \tag{A.11}$$

hence $H_0\mathrm{e}^{-\mathrm{i}tA_0} = \mathrm{e}^{-\mathrm{i}t(A_0-2\mathrm{i})}H_0$. Now, for $f \in H^2(d)$,

$$\begin{aligned}H_0 f(A_0) &= \int_{-\infty}^{\infty} H_0 \mathrm{e}^{\mathrm{i}tA_0}\hat{f}(t)dt \\ &= \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}t(A_0-2\mathrm{i})}H_0\hat{f}(t)dt = f(A_0 - 2\mathrm{i})H_0 ,\end{aligned}$$

where the last step is justified by the above-mentioned property of the Hardy class functions. □

LEMMA A.4 *Let $f' \in H^2(d)$ with $d > 2$ and $g \in C_0^\infty(\mathbb{R})$. Then*

$$(f(A) - f(A_0))g(H_0) \in J_1 . \tag{A.12}$$

PROOF: As already mentioned, the Fourier transform of

$$f'(\lambda) = \int_{-\infty}^{\infty} dt\, \mathrm{e}^{i\lambda t}\widehat{f'}(t)$$

is bounded as

$$|\widehat{f'}(t)| \le C\mathrm{e}^{-y|t|} \tag{A.13}$$

for any $y < d$. We represent f as

$$f(\lambda) = f(0) + \int_{-\infty}^{\infty} dt \left(\frac{e^{i\lambda t} - 1}{it} \right) \widehat{f'}(t)$$

and write

$$\frac{1}{it}(e^{iAt} - e^{iA_0 t}) = \frac{1}{t} \int_0^t ds\, e^{iA(t-s)}(A - A_0) e^{iA_0 s},$$
$$e^{iA_0 s} g(H_0) = g(H_0 e^{-2s}) e^{iA_0 s},$$

which follows from (A.11). Applying theorem XI.20 of [20] to

$$(A - A_0) g(H_0 e^{-2s}) = \left(w(x) p - \frac{i}{2} w'(x) \right) g(H_0 e^{-2s}),$$

where $w(x) = v(x) - x$, one finds

$$\left\| (A - A_0) g(H_0 e^{-2s}) \right\|_1 \le C_\delta \left(e^{s(\frac{3}{2}+\delta)} + e^{s(\frac{1}{2}+\delta)} \right) \tag{A.14}$$

for any $\delta > \frac{1}{2}$. We obtain $\|t^{-1}(e^{iAt} - e^{iA_0 t}) g(H_0)\|_1 \le C(1 + e^{\tilde{d} t})$ with $\tilde{d} = \frac{3}{2} + \delta$. Picking δ so that $\tilde{d} < d$, we obtain the claim from equation (A.13). □

The following lemma will be useful.

LEMMA A.5

$$\left\| H_0 (H_0 + 1)^{-2} (A_0 - z)^{-2} \right\|_1 \le C |\operatorname{Im} z|^{-2}. \tag{A.15}$$

PROOF: It suffices to prove the claim for $|\operatorname{Im} z|$ large enough since

$$\left\| (A_0 - z + iy)(A_0 - z)^{-1} \right\| \le C |\operatorname{Im} z|^{-2}$$

for small $|\operatorname{Im} z|$. We shall do that for $|\operatorname{Im} z| > 4$. By the pull-through formula, equation (A.10), we compute

$$\begin{aligned} &H_0 (A_0 - z)^{-1} \\ &\quad = (A_0 - z - 2i)^{-1} H_0 \\ &\quad = (A_0 - z - 2i)^{-1} \left(H_0^2 + 2H_0 + 1 \right) H_0 (H_0 + 1)^{-2} \\ &\quad = \left[H_0^2 (A_0 - z + 2i)^{-1} + 2H_0 (A_0 - z)^{-1} + (A_0 - z - 2i)^{-1} \right] H_0 (H_0 + 1)^{-2}. \end{aligned}$$

We multiply this expression from the left by $(H_0 + 1)^{-2}$ and from the right by $(A_0 - z)^{-2}$, so as to obtain the bound

$$\begin{aligned} &\left\| H_0 (H_0 + 1)^{-2} (A_0 - z)^{-2} \right\|_1 \le \\ &\qquad \sum_{k=-1}^{1} \left\| (A_0 - z + 2ki)^{-1} H_0 (H_0 + 1)^{-2} (A_0 - z_2)^{-1} \right\|_1. \end{aligned}$$

Equation (A.1) now yields $\|H_0^{1/2} (H_0 + 1)^{-1} (A_0 - z)^{-1}\|_2 = (2|\operatorname{Im} z|)^{-1/2}$. Hence (A.15) follows from the Hölder inequality. □

LEMMA A.6 *For $g \in C_0^\infty(0,\infty)$ we have*

$$\sup_{a\in\mathbb{R}} \|(A-a\pm \mathrm{i})^{-2} g(H)\|_1 < \infty\,. \tag{A.16}$$

In particular, for any $f \in C^\infty(\mathbb{R})$ with $f(x)(x+\mathrm{i})^2$ bounded,

$$f(A)g(H) \in \mathcal{J}_1\,. \tag{A.17}$$

PROOF: Since $g(H_0)H_0^{-1}(H_0+1)^2$ is bounded, by (A.15) the bound holds for A_0 and H_0 in place of A and H. We first undo the replacement in A and write

$$\begin{aligned}(A-a\pm \mathrm{i})^{-2} g(H_0) = {} & (A-a\pm \mathrm{i})^{-2}\phi(x) g(H_0) \\ & + (A-a\pm \mathrm{i})^{-2}(1-\phi(x))g(H_0)\,,\end{aligned}$$

where $\phi \in C_0^\infty[0,\infty)$ has $v(x) = x$ on $\mathrm{supp}(1-\phi)$. Then $\phi(x)g(H_0) \in J_1$ (see [20, theorem XI.20]). For the second term on the right-hand side we write, dropping a,

$$(A+\mathrm{i})^{-2}(1-\phi(x))(A_0+\mathrm{i})^2 \cdot (A_0+\mathrm{i})^{-2} g(H_0)\,.$$

Since the last factor is trace class, we are left with showing that the first factor is bounded. This follows from

$$(1-\phi)(A_0+\mathrm{i})^2 = (A+\mathrm{i})^2(1-\phi) - (A+\mathrm{i})[\phi, A_0] - [\phi, A_0](A+\mathrm{i})\,,$$

where $[\phi, A] = \mathrm{i}x\phi'(x)$ is bounded.

The bound (A.16) clearly also holds for

$$(A+\mathrm{i})^{-2} J g(H_0) J^* = J(A+\mathrm{i})^{-2} g(H_0) J^*$$

and hence, by (A.6), also in the form stated in the claim. □

Acknowledgments. This work is supported in part by the Israel Science Foundation, the fund for promotion of research at the Technion, the Texas Advanced Research Program, NSF Grant PHY-9971149, and the Swiss National Science Foundation. G.M.G. thanks T. Spencer for hospitality at the Institute for Advanced Study, where part of this work was done. Also, we would like to acknowledge the careful proofreading of the editor.

Bibliography

[1] Aleiner. L. L.; Andreev, A. V. Adiabatic charge pumping in almost open dots. *Phys. Rev. Lett.* **81** (1998), 1286.

[2] Amrein, W. O.; Boutet de Monvel, A.; Georgescu, V. C_0-groups, commutator methods and spectral theory of N-body Hamiltonians. Progress in Mathematics, 135. Birkhäuser, Basel, 1996.

[3] Avron, J. E.; Elgart, A. Adiabatic theorem without a gap condition. *Comm. Math. Phys.* **203** (1999), no. 2, 445–463.

[4] Avron, J. E.; Elgart, A.; Graf, G. M.; Sadun, L. Optimal quantum pumps. *Phys. Rev. Lett.* **87** (2001), 236601.

[5] Avron, J. E.; Elgart, A.; Graf, G. M.; Sadun, L. Time-energy coherent states and adiabatic scattering. *J. Math. Phys.* **43** (2002), no. 7, 3415–3424.

[6] Bornemann, F. *Homogenization in time of singularly perturbed mechanical systems*. Lecture Notes in Mathematics, 1687. Springer, Berlin, 1998.

[7] Brouwer, P. W. Scattering approach to parametric pumping. *Phys. Rev. B* **58** (1998), 10135.

[8] Büttiker, M.; Thomas, H.; Prêtre, A. Current partition in multi-probe conductors in the presence of slowly oscillating external potentials. *Z. Phys. B* **94** (1994), 133–137.

[9] Combes, J. M.; Thomas, L. Asymptotic behaviour of eigenfunctions for multiparticle Schrödinger operators. *Comm. Math. Phys.* **34** (1973), 251–270.

[10] Davies, E. B. *Spectral theory of differential operators*. Cambridge University Press, Cambridge, 1995.

[11] Dereziński, J.; Gérard, C. *Scattering theory of classical and quantum N-particle systems*. Springer, Berlin, 1997.

[12] Dollard, J. D.; Friedman, C. N. Scattering of a beam of particles by a potential. *J. Math. Phys.* **20** (1979), no. 8, 1727–1730.

[13] Hunziker, W.; Sigal, I. M. Time-dependent scattering theory of N-body quantum systems. *Rev. Math. Phys.* **12** (2000), no. 8, 1033–1084.

[14] Hunziker, W.; Sigal, I. M.; Soffer, A. Minimal escape velocities. *Comm. Partial Differential Equations* **24** (1999), no. 11-12, 2279–2295.

[15] Ivanov, D. A.; Lee, H. W.; Levitov, L. S. Coherent states of alternating current. *Phys. Rev. B* **56** (1997), 6839–6850.

[16] Jensen, A.; Mourre, E.; Perry, P. Multiple commutator estimates and resolvent smoothness in quantum scattering theory. *Ann. Inst. H. Poincaré Phys. Théor.* **41** (1984), no. 2, 207–225.

[17] Levitov, L. S.; Lee, H.; Lesovik, G. B. Electron counting statistics and coherent states of electric current. *J. Math. Phys.* **37** (1996), no. 10, 4845–4866.

[18] Martin, P. A.; Sassoli de Bianchi, M. On the low- and high-frequency limit of quantum scattering by time-dependent potentials. *J. Phys. A* **28** (1995), no. 8, 2403–2427.

[19] Martinez, A.; Nakamura, S. Adiabatic limit and scattering. *C. R. Acad. Sci. Paris Sér. I Math.* **318** (1994), no. 12, 1153–1158.

[20] Reed, M.; Simon, B. *Methods of modern mathematical physics. III. Scattering theory*. Academic, New York, 1979.

[21] Shutenko, T. A.; Aleiner, I. L.; Altshuler, B. L. Mesoscopic fluctuations of adiabatic charge pumping in quantum dots. *Phys. Rev. B* **61** (2000), no. 15, 10366–10375.

[22] Simon, B. *Trace ideals and their applications*. Cambridge University Press, New York, 1979.

[23] Sjöstrand, J.; Zworski, M. Complex scaling and the distribution of scattering poles. *J. Amer. Math. Soc.* **4** (1991), no. 4, 729–769.

[24] van Kampen, N. G. A discussion on linear response theory. *Physica Norvegica* **5** (1971), 279.

[25] Yafaev, D. R. *Mathematical scattering theory. General theory*. Translations of Mathematical Monographs, 105. American Mathematical Society, Providence, R.I., 1992.

JOSEPH E. AVRON
Technion—Israel Institute of Technology
Department of Physics
32000 Haifa
ISRAEL
E-mail: `avron@physics.technion.ac.il`

ALEXANDER ELGART
Stanford University
Department of Mathematics
Building 380
Stanford, CA 94305-2125
E-mail: `elgart@stanford.edu`

GIAN MICHELE GRAF
ETH Hönggerberg
Theoretische Physik
8093 Zürich
SWITZERLAND
E-mail: gmgraf@itp.phys.ethz.ch

LORENZO SADUN
University of Texas at Austin
Department of Mathematics
1 University Station C1200
Austin, TX 78712-0257
E-mail: sadun@math.texas.edu

KAI SCHNEE
ETH Zürich
Theoretische Physik
8093 Zürich
SWITZERLAND
E-mail: schnee@itp.phys.ethz.ch

Received March 2003.