Lower bounds for the conductivities of correlated quantum systems

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(Dated: February 5, 2008)

We show how one can obtain a lower bound for the electrical, spin or heat conductivity of correlated quantum systems described by Hamiltonians of the form $H = H_0 + gH_1$. Here $H_0$ is an interacting Hamiltonian characterized by conservation laws which lead to an infinite conductivity for $g = 0$. The small perturbation $gH_1$, however, renders the conductivity finite at finite temperatures. For example, $H_0$ could be a continuum field theory, where momentum is conserved, or an integrable one-dimensional model while $H_1$ might describe the effects of weak disorder. In the limit $g \to 0$, we derive lower bounds for the relevant conductivities and show how they can be improved systematically using the memory matrix formalism. Furthermore, we discuss various applications and investigate under what conditions our lower bound may become exact.

PACS numbers: 72.10.Bg, 05.60.Gg, 75.40.Gb, 71.10.Pm

I. INTRODUCTION

Transport properties of complex materials are not only important for many applications but are also of fundamental interest as their study can give insight into the nature of the relevant quasi particles and their interactions.

Compared to thermodynamic quantities, the transport properties of interacting quantum systems are notoriously difficult to calculate even in situations where interactions are weak. The reason is that conductivities of non-interacting systems are usually infinite even at finite temperature, implying that even to lowest order in perturbation theory an infinite resummation of a perturbative series is mandatory. To lowest order this implies that one usually has to solve an integral equation, often written in terms of (quantum-) Boltzmann equations or – within the Kubo formalism – in terms of vertex equations. The situation becomes even more difficult if the interactions are so strong that an expansion around a non-interacting system is not possible. Also numerically, the calculation of zero-frequency conductivities of strongly interacting clean systems is a serious challenge and even for one-dimensional systems reliable calculations are available for high temperatures only\cite{1,2,3,4,5,6}.

Variational estimates, e.g., for the ground state energy, are powerful theoretical techniques to obtain rigorous bounds on physical quantities. They can be used to guide approximation schemes to obtain simple analytic estimates and are sometimes the basis of sophisticated numerical methods like the density matrix renormalization group\cite{7,8}.

Taking into account both the importance of transport quantities and the difficulties involved in their calculation it would be very useful to have general variational bounds for transport coefficients.

A well known example where a bound for transport quantities has been derived is the variational solution of the Boltzmann equation, discussed extensively by Ziman\cite{9}. The linearized Boltzmann equation in the presence of a static electric field can be written in the form

$$\epsilon E V_k \frac{d \varphi_k}{d \epsilon_k} = \sum_{k'} W_{k,k'} \varphi_{k'}$$

(1)

where $W_{k,k'}$ is the integral kernel describing the scattering of quasiparticles and we have linearized the Boltzmann equation around the Fermi (or Bose) distribution $f_k^{0} = f^0(\epsilon_k)$ using $f_k = f_k^{0} - \frac{d \varphi_k}{d \epsilon_k}$. Therefore, the current is given by $I = -e \sum_k v_k \frac{d \varphi_k}{d \epsilon_k}$ and the dc conductivity is determined from the inverse of the scattering matrix $W$ using $\sigma = -e^2 \sum_{kk'} v_k v_{k'} W_{k,k'}^{-1} \frac{d \varphi_k}{d \epsilon_k}$. It is easy to see that this result can be obtained by maximizing a functional $\int_{\Phi}$ with

$$\sigma = e^2 \max_{\Phi} F[\Phi] \geq e^2 \max_{\Phi} F \left[ \sum_i \alpha_i \phi_i \right]$$

(2)

$$F[\Phi] = \frac{2 \left( \sum_k v_k \varphi_k \frac{d \varphi_k}{d \epsilon_k} \right)^2}{\sum_{k,k'} \left( \varphi_k - \varphi_{k'} \right)^2 W_{k,k'}}$$

where we used that $\sum_{k'} W_{k,k'} = 0$ reflecting the conservation of probability. The variational formula (2) is actually closely related to the famous H-theorem of Boltzmann which states that entropy always increases upon scattering.

A lower bound for the conductivity can be obtained by varying $\Phi$ only in a subspace of all possible functions. This allows for example to obtain analytically good estimates for conductivities without inverting an infinite dimensional matrix or, equivalently, solving an integral equation, see Ziman’s book for a large number of examples\cite{9}.

The applicability of Eq. (2) is restricted to situations where the Boltzmann equation is valid and bounds for the conductivity in more general setups are not known. However, for ballistic systems with infinite conductivity it is possible to get a lower bound for the so-called Drude weight. Mazumdar\cite{10} and later Suzuki\cite{12} considered situations where the presence of conservation laws prohibits the decay of certain correlation functions in the
long time limit. In the context of transport theory their result can be applied to systems (see Appendix A for details) where the finite-temperature conductivity $\sigma(\omega, T)$ is infinite for $\omega = 0$ and characterized by a finite Drude weight $D(T) > 0$ with

$$\text{Re} \sigma(\omega, T) = \pi D(T) \delta(\omega) + \sigma_{\text{reg}}(\omega, T).$$

Such a Drude weight can arise only in the presence of exact conservation laws $C_j$ with $[H, C_j] = 0$. Suzuki\cite{Suzuki1971}, showed that the Drude weight can be expressed as a sum over all $C_j$

$$D = \frac{1}{V} \sum_{j=0}^{\infty} \frac{\langle C_j J \rangle^2}{\langle C_j \rangle^2} \geq \frac{1}{V} \sum_{j=0}^{N} \frac{\langle C_j J \rangle^2}{\langle C_j \rangle^2},$$

where $J$ is the current associated with $\sigma$. For convenience a basis in the space of $C_j$ has been chosen such that $\langle C_i C_j \rangle = 0$ for $i \neq j$. More useful than the equality in Eq. (4) is often the inequality\cite{Suzuki1971} which is obtained when the sum is restricted to a finite subset of conservation laws. Such a finite sum over simple expectation values can often be calculated rather easily using either analytical or numerical methods. The Mazur inequality has recently been used heavily\cite{ Yan2014, Yan2015, Yan2016, Yan2017} to discuss the transport properties of one-dimensional systems.

Model systems, due to their simplicity, often exhibit symmetries not shared by real materials. For example, the heat conductivity of idealized one-dimensional Heisenberg chains is infinite at arbitrary temperature as the heat current is conserved. However, any additional coupling (next-nearest neighbor, inter-chain, disorder, phonon,...) renders the conductivity finite\cite{Yan2014, Yan2015, Yan2016, Yan2017}. If these perturbations are weak, the heat conductivity is, however, large as observed experimentally\cite{Yan2021, Yan2022}. For a more general example, consider an arbitrary translationally invariant continuum field theory. Here momentum is conserved which usually implies that the conductivity is infinite for this model. In real materials momentum decays by Umklapp scattering or disorder rendering the conductivity finite. It is obviously desirable to have a reliable method to calculate transport in such situations. In this work we consider systems with the Hamiltonian

$$H = H_0 + g H_1,$$

where for $g = 0$ the relevant heat-, charge- or spin-conductivity is infinite and characterized by a finite Drude weight given by Eq. (4). As discussed above, $H_0$ might be an integrable one-dimensional model, a continuum field theory, or just a non-interacting system. The term $g H_1$ describes a (weak) perturbation which renders the conductivity finite, e.g. due to Umklapp scattering or disorder, see Fig. 1. Our goal is to find a variational lower bound for conductivities in the spirit of Eq. (2) for this very general situation, without any requirement on the existence of quasi particles. For technical reasons (see below) we restrict our analysis to situations where $H$ is time reversal invariant.

In the following, we first describe the general setup and introduce the memory matrix formalism, which allows us to formulate an inequality for transport coefficients for weakly perturbed systems. We will argue that the inequality is valid under the conditions which we specify. Finally, we investigate under which conditions the lower bounds become exact and briefly discuss applications of our formula.

II. SETUP

Consider the local density $\rho(x)$ of an arbitrary physical quantity which is locally conserved, thus obeying a continuity equation

$$\partial_t \rho + \nabla j = 0.$$

Transport of that quantity is described by the dc conductivity $\sigma$ which is the response of the current to some external field $E$ coupling to the current,

$$\langle J \rangle = \sigma E,$$

where $J = \int j(x) \, dx$ is the total current and $\langle J \rangle$ its expectation value. Note that $J$ can be an electrical-, charge-, spin-, or heat current and $E$ the corresponding conjugate field depending on the context. The dynamic conductivity $\sigma(z)$ is given by Kubo’s formula, see Eq. (A1). We are interested in the dc conductivity $\sigma = \lim_{\omega \to 0} \sigma(z = \omega + i0)$.

Starting from the Hamiltonian (5) we consider a system where $H_0$ possesses a set of exact conservation laws $\{C_i\}$ of which at least one correlates with the current, $\langle JC_i \rangle \neq 0$. Without loss of generality we assume $\langle C_i C_j \rangle = 0$ for $i \neq j$. For $g = 0$ the Drude weight $D$ defined by Eq. (4) is given by Eq. (4). We can split up the current under consideration into a part which is parallel to the $C_i$ and one that is orthogonal,

$$J = J_{//} + J_{\bot},$$

with $J_{//} = \sum_i \frac{\langle C_i J \rangle}{\langle C_i \rangle} C_i$, which results in a separation of the conductivity;

$$\sigma(z) = \sigma_{//}(z) + \sigma_{\bot}(z).$$

FIG. 1: For $g = 0$ a Drude peak shows up in the conductivity, resulting from exact conservation laws. For $g \neq 0$ the Drude peak broadens and the dc conductivity becomes finite.
Since the conductivity $\sigma(z)$ is given by a current-current correlation function and the current $J_0 (J_\perp)$ is diagonal (off-diagonal) in energy, cross-correlation functions $\langle \langle J_i; J_j \rangle \rangle$ vanish in Eq. (6).

According to Eq. (4), the Drude peak of the unperturbed system, $g = 0$, arises solely from $J_\parallel$:

$$\text{Re} \sigma_\parallel(\omega) = \pi D \delta(\omega), \quad (7)$$

while $\sigma_\perp(z)$ appears in Eq. (3) as the regular part, $\text{Re} \sigma_\perp(\omega) = \text{Re} g_{\delta}(\omega)$.

In this work we will focus on $\sigma_\parallel(\omega)$, since the small perturbation is not going to affect $\sigma_\perp(\omega)$ much (which is assumed to be free of singularities here, see section [11]) while $\sigma_\parallel(\omega = 0)$ diverges for $g \to 0$, see Fig. [1] As we are interested in the small $g$ asymptotics only, we may neglect the contribution $\sigma_\perp(0)$ to the dc conductivity. Hence we set $J = J_\parallel$ and $\sigma(\omega) = \sigma_\parallel(\omega)$ in the following.

### III. MEMORY MATRIX FORMALISM

We have seen that certain conservation laws of $H_0$ play a crucial role in determining the conductivity of both the unperturbed and the perturbed system. In the presence of a small perturbation $gH_1$, these modes are not conserved anymore but at least some of them decay slowly. Typically, the conductivity of the perturbed system will be determined by the dynamics of these slow modes. To separate the dynamics of the slow modes from the rest, it is convenient to use a hydrodynamic approach based on the projection of the dynamics onto these slow modes. In this section we will therefore review the so-called memory matrix formalism, introduced by Mori and Zwanzig for this purpose. In the next section we will show that this approach can be used to obtain a lower bound for the dc conductivity for small $g$.

We start by defining a scalar product in the space of quantum mechanical operators,

$$\langle A|B \rangle = \int_0^\beta d\lambda \langle A^\dagger B(i\lambda) \rangle - \beta \langle A^\dagger \rangle \langle B \rangle \quad (8)$$

As the next step we choose a – for the moment – arbitrary set of operators $\{C_i\}$. In most applications, the $C_i$ are the relevant slow modes of the system. For notational convenience, we assume that the $\{C_i\}$ are orthonormalized,

$$\langle C_i | C_j \rangle = \delta_{ij}. \quad (9)$$

In terms of these we may define the projector $P$ onto (and $Q$ away from) the space spanned by these 'slow' modes

$$P = \sum_i |C_i\rangle \langle C_i| = 1 - Q.$$ 

We assume that $C_1$ is the current we are interested in,

$$|J\rangle \equiv |C_1\rangle.$$ 

The time evolution is given by the Liouville-(super)operator

$$L = [H, .] = L_0 + gL_1$$

with $(LA|B) = (A|LB) = (A|L|B)$, and the time evolution of an operator may be expressed as $|A(t)\rangle = e^{iHt} A e^{-iHt} = e^{iLt} |A\rangle$. With these notions, one obtains the following simple, yet formal expression for the conductivity:

$$\sigma(\omega) = \left( J \left| \frac{i}{\omega - L} \right| J \right) = \left( C_1 \left| \frac{i}{\omega - L} \right| C_1 \right).$$

Using a number of simple manipulations, one can show that the conductivity can be expressed as the $(1,1)$-component of the inverse of a matrix

$$\sigma(\omega) = (M(\omega) + iK - i\omega)^{-1}.$$

where

$$M_{ij}(\omega) = \left( \hat{C}_i \left| \frac{i}{\omega - L} \right| C_j \right) \quad (11)$$

is the so-called memory matrix and

$$K_{ij} = \left( \hat{C}_i Q \left| \frac{i}{\omega - L} \right| C_j \right) \quad (12)$$

a frequency independent matrix. The formal expression for the conductivity is exact, and completely general, i.e. valid for an arbitrary choice of the modes $C_i$ (they do not even have to be 'slow'). Only $C_1 = J$ is required. However, due to the projection operators $Q$, the memory matrix is in general difficult to evaluate. It is when one uses approximations to $M$ that the choice of the projectors becomes crucial (see below).

Obviously, the dc conductivity is given by the $(1,1)$-component of

$$(M(0) + K)^{-1}. \quad (13)$$

More generally, the $(m,n)$-component of Eq. (13) describes the response of the 'current' $C_m$ to an external field coupling solely to $C_n$. We note, that since a matrix of transport coefficients has to be positive (semi)definite, this also holds for the matrix $M(0) + K$.

To avoid technical complications associated with the presence of $K$ we restrict our analysis in the following to time reversal invariant systems and choose the $C_i$ such, that they have either signature $+1$ or $-1$ under time reversal $\Theta$. In the dc limit, $\omega = 0$, components of Eq. (13) connecting modes of different signatures vanish. Thus, $M(0) + K$ is block-diagonal with respect to the time reversal signature, and consequently we can restrict our analysis to the subspace of slow modes with the same signature as $C_1$. However, if $C_m$ and $C_n$ have the same signature, then $(C_m|C_n) = 0$, and thus $K$ vanishes on this restricted space. The dc conductivity therefore takes the form

$$\sigma = (M(0))^{-1}_{11}. \quad (14)$$
IV. CENTRAL CONJECTURE

To obtain a controlled approximation to the memory matrix in the limit of small $g$, it is important to identify the relevant slow modes of the system. For the $C_i$, we choose quantities which are conserved by $H_0$, $[H_0, C_i] = 0$, such that $\dot{C}_i = i g [H_1, C_i]$ is linear in the small coupling $g$. As argued below, we require that the singularities of correlation functions of the unperturbed system are exclusively due to exact conservation laws $C_i$, i.e. that the Drude peak appearing in Eq. (3) is the only singular contribution. Furthermore, we choose $J = J_0 = C_1$ and consider only $C_i$ with the same time reversal signature as $J$, as discussed in the previous section.

To formulate our central conjecture we introduce the following notions. We define $M_n(\omega)$ as the (exact) $n \times n$ memory matrix obtained by setting up the memory matrix formalism for the first $n$ slow modes $\{C_i, i = 1, \ldots, n\}$. Note that the definitions of the relevant projectors $P$ and $Q$ also depend on this choice, and that for any choice of $n$ one gets $\sigma = (M_n^{-1})_{11}$. We now introduce the approximate memory matrix $\tilde{M}_n$ motivated by the following arguments: $\dot{C}_i$ is already linear in $g$, therefore in Eq. (11) we approximate $L$ by $L_0$ and replace $\langle \cdot \rangle$ by $\langle \cdot \rangle_0$ as we evaluate the scalar product with respect to $H_0$. As $L_0|C_i\rangle = 0$ and $\langle C_j|\dot{C}_i\rangle = 0$ due to time reversal symmetry, one has $L_0Q = 1$ and $Q|\dot{C}_i\rangle = |\dot{C}_i\rangle$ and therefore the projector $Q$ does not contribute within this approximation. We thus define the $n \times n$ matrix $\tilde{M}_n$ by

$$\tilde{M}_{n,ij} = \lim_{\omega \to 0} \left( \dot{C}_i | i \omega - L_0 | C_j \right)_0$$

Note that $\tilde{M}_n$ is a submatrix of $\tilde{M}_m$ for $m > n$ and that for $m > n$ the approximate expression for the conductivity $\sigma \approx (M_n^{-1})_{11}$ does depend on $n$ while $(M_m^{-1})_{11}$ is independent of $n$. A much simpler, alternative derivation for $\tilde{M}_1$ is given in Appendix B where the validity of this formula is also discussed.

The central conjecture of our paper is, that for small $g$, $(\tilde{M}_n^{-1})_{11}$ gives a lower bound to the dc conductivity, or, more precisely,

$$\sigma_{1/g^2} = (\tilde{M}_n^{-1})_{11} \geq \cdots \geq (\tilde{M}_m^{-1})_{11} \geq \cdots \geq \tilde{M}_1^{-1}.$$  \hspace{1cm} (16)

Here $\sigma_{1/g^2} = (1/g^2) \lim_{g \to 0} g^2 \sigma$ denotes the leading term $\propto 1/g^2$ in the small-$g$ expansion of $\sigma$. Note that $\tilde{M}_n \propto g^2$ by construction. $\tilde{M}_\infty$ is the approximate memory matrix where all conservation laws have been included. In some special situations, discussed in Ref. [6], one has $\sigma \sim 1/g^4$ and therefore $\sigma_{1/g^2} = \infty$.

A special case of the inequality above is Eq. (16) in appendix B as the scattering rate $\Gamma/\chi$ may be expressed as $\Gamma/\chi = \tilde{M}_1$.

Two steps are necessary to prove Eq. (16). The simple part is actually the inequalities in Eq. (16). They are a consequence of the fact that the matrices $M_n$ are all positive definite and that $\tilde{M}_n$ is a submatrix of $\tilde{M}_m$ for $m \geq n$. More difficult to prove is that the first equality in (16) holds. To show this we will need an additional assumption, namely, that the regular part of all correlation functions (to be defined below) remains finite in the limit $g \to 0$, $\omega \to 0$. In this case, the perturbative expansion around $\tilde{M}_\infty$ in powers of $g$ is free of singularities at finite temperature (which is not the case for $M_{n<\infty}$). This in turn implies that $\lim_{g \to 0} M_{n\infty}/g^2 = M_{n\infty}/g^2$ and therefore $\sigma_{1/g^2} = (\tilde{M}_n^{-1})_{11}$.

Next, we present the two parts of the proof.

A. Inequalities

We start by investigating the $(1,1)$-component of the inverse of the positive definite symmetric matrix $\tilde{M}_\infty$. It is convenient to write the inverse as

$$\left(\tilde{M}_{\infty}^{-1}\right)_{11} = \max_{\varphi} \frac{(\varphi^T e_1)^2}{\varphi^T \tilde{M}_\infty \varphi}$$

where $e_1$ is the first unit vector. The same method is used to derive Eq. (2) in the context of the Boltzmann equation. The maximum is obtained for $\varphi = \tilde{M}_{\infty}^{-1} e_1$. By restricting the variational space to the first $n$ components of $\varphi$, we reproduce the submatrix $\tilde{M}_n$ of $\tilde{M}_{\infty}$ and obtain

$$\left(\tilde{M}_n^{-1}\right)_{11} \geq \max_{\varphi = \sum_i \lambda_i e_i} \frac{(\varphi^T e_1)^2}{\varphi^T \tilde{M}_\infty \varphi} = (\tilde{M}_m^{-1})_{11}$$

By choosing different values for $m$ and $n < m$, this proves all inequalities appearing in (16).

B. Expansion of the memory matrix

We proceed by expanding the exact memory matrix $M_n$, where $P_n = 1 - Q_n$ is a projector on the first $n$ conservation laws, in powers of $g$. Using that $LQ_n = L_0 + g L_1 Q_n$, we obtain the geometric series

$$M_{n,ij}(\omega) = \sum_{k=0}^{\infty} g^k \left( \dot{C}_i | Q_n \omega - L_0 | L_1 Q_n \omega - L_0 \right)^k | \dot{C}_j \rangle.$$ \hspace{1cm} (18)

Note that this is not a full expansion in $g$, as the scalar product is defined with respect to the full Hamiltonian $H = H_0 + g H_1$. We will turn to the discussion of the remaining $g$-dependence later.

In general, one can expand

$$L_1 = \sum_{m,n} \lambda_{mn} | A_m \rangle | A_n \rangle$$

with

$$\tilde{M}_{n,ij}(\omega) = \sum_{k=0}^{\infty} g^k \left( \dot{C}_i | Q_n \omega - L_0 | L_1 Q_n \omega - L_0 \right)^k | \dot{C}_j \rangle.$$ \hspace{1cm} (18)

Note that this is not a full expansion in $g$, as the scalar product is defined with respect to the full Hamiltonian $H = H_0 + g H_1$. We will turn to the discussion of the remaining $g$-dependence later.
in terms of some basis $A_{\alpha}$ in the space of operators. Therefore Eq. (18) can be written as a sum over products of terms with the general structure

$$ \left( A \left| Q_n \frac{1}{\omega - L_0} \right| B \right).$$

(19)

In the following we would like to argue that such an expansion is regular for $n = \infty$ if all conservation laws have been included in the definition of $Q$. As argued in Appendix B we have to investigate whether the series coefficients in Eq. (18) diverge for $\omega \to 0$. The basis of our argument is the following: as $Q_{\infty}$ projects the dynamics to the space perpendicular to all of the conservation laws, the associated singularities are absent in Eq. (19) and therefore the expansion of $M_{\infty}$ is regular.

To show this more formally, we split up $B = B_\parallel + B_\perp$ in (18) into a component parallel and one perpendicular to the space of all conserved quantities, $\langle B_\parallel \rangle = P_{\infty} \langle B \rangle$. With this notation, the action of $L_0$ becomes more transparent:

$$ \frac{1}{\omega - L_0} \langle B \rangle = \frac{1}{\omega} \langle B_\parallel \rangle + \frac{1}{\omega - L_0} \langle B_\perp \rangle.$$

(20)

As we assume that all divergencies can be traced back to the conservation laws, we take the second term to be regular. It is only the first term which leads in Eq. (19) to a divergence for $\omega \to 0$, provided that $\langle A(Q_n | B_\parallel) \rangle$ is finite. If we consider the perturbative expansion of $M_{n<\infty}$, where $P_n = 1 - Q_n$ projects only to a subset of conserved quantities, then finite contributions of the form $\langle A(Q_n | B_\parallel) \rangle$ exist and the perturbative series in $g$ will be singular (see also Appendix B). Considering $M_{\infty}$, however, $Q_{\infty}$ projects out all conservation laws and therefore by construction $Q_{\infty} \langle B_\parallel \rangle = Q_{\infty} P_{\infty} \langle B \rangle = 0$. Thus the first term in (20) does not contribute in (19) for $n = \infty$ and the expansion (18) of $M_{\infty}$ is therefore regular.

The only remaining part of our argument is to show that in the limit $g \to 0$ one can safely replace $(\ldots)$ by $(\ldots)_0$. Here it is useful to realize that $\langle A | B \rangle$ can be interpreted as a (generalized) static susceptibility. In the absence of a phase transition and at finite temperatures, susceptibilities are smooth, non-singular functions of the coupling constants and therefore we do not expect any further singularities from this step. If we define a phase transition by a singularity in some generalized susceptibility, then the statement that singularities are regular in the absence of phase transitions even becomes a mere tautology.

Combining all arguments, the expansion (18) of $M_{\infty}(\omega \to 0)$ is regular, and using $\langle C_\alpha | Q_{\infty} = \langle C_\alpha \rangle$ [see discussion before Eq. (15)] its leading term, $k = 0$ is given by $M_{\infty}$. We therefore have shown the missing first equality of our central conjecture (16).

V. DISCUSSION

In this paper we have established that in the limit of small perturbations, $H = H_0 + gH_1$, lower bounds to dc conductivities may be calculated for situations where the conductivity is infinite for $g = 0$. In the opposite case, when the conductivity is finite for $g = 0$, one can use naive perturbation theory to calculate small corrections to $\sigma$ without further complications.

The relevant lower bounds are directly obtained from the memory matrix formalism. Typically26,27,28 one has to evaluate a small number of correlation functions and to invert small matrices. The quality of the lower bounds depends decisively on whether one has been able to identify the ‘slowest’ modes in the system.

There are many possible applications for the results presented in this paper. The mostly considered situation is the case where $H_0$ describes a non-interacting system. For situations where the Boltzmann equation can be applied, it has been pointed out a long time ago by Belitz29 that there is a one-to-one relation of the memory matrix calculation to a certain variational Ansatz to the Boltzmann equation, see Eq. (2). In this paper we were able to generalize this result to cases where a Boltzmann description is not possible. For example, if $H_0$ is the Hamiltonian of a Luttinger liquid, i.e. a non-interacting bosonic system, then typical perturbations are of the form $\cos \phi$ for which a simple transport theory in the spirit of a Boltzmann or vertex equation does not exist to our knowledge.

Another class of applications are systems where $H_0$ describes an interacting system, e.g. an integrable one-dimensional model30 or some non-trivial quantum-field theory31. In these cases it can become difficult to calculate the memory matrix and one has to resort to use either numerical or field-theoretical methods32 to obtain the relevant correlation functions.

An important special case are situations where $H_0$ is characterized by a single conserved current with the proper symmetries, i.e. with overlap to the (heat-, spin- or charge-) current $J$. For example, in a non-trivial continuum field theory $H_0$, interactions lead to the decay of all modes with exception of the momentum $P$. In this case the momentum relaxation and therefore the conductivity at finite $T$ is determined by small perturbations $gH_1$ like disorder or Umklapp scattering which are present in almost any realistic system. As $M_{\infty} = M_1$ in this case, our results suggest that for small $g$ the conductivity is exactly determined by the momentum relaxation rate $\frac{\partial}{\partial \omega} \langle P | (\omega - L_0)^{-1} | P \rangle$, $\sigma = \frac{\chi_{P,J}}{M_{PP}}$ for $g \to 0$.

(21)

Here we used that $J_0 = \langle P | J \rangle / \langle P | P \rangle$ with $\chi_{P,J} = \langle P | J \rangle$ and we have restored all factors which arise if the normalization condition (3) is not used. In Appendix C we check numerically that this statement is valid for a realistic example within the Boltzmann equation approach.
A number of assumptions entered our arguments. The strongest one is the restriction that all relevant singularities arise from exact conservation laws of $H_0$. We assumed that the regular parts of correlation functions are finite for $\omega = 0$. There are two distinct scenarios in which this assumption does not hold. First, in the limit $T \to 0$, often scattering rates vanish which can lead to divergencies of the nominally regular parts of correlation functions. Furthermore, at $T = 0$ even infinitesimally small perturbations can induce phase transitions -- again a situation where our arguments fail. Therefore our results are not applicable at $T = 0$. Second, finite temperature transport may be plagued by additional divergencies for $\omega \to 0$ not captured by the Drude weight. In some special models, for instance, transport is singular even in the absence of exactly conserved quantities (e.g. non-interacting phonons in a disordered crystal). In all cases known to us, these divergencies can be traced back to the presence of some slow modes in the system (e.g. phonons with very low momentum). While we have not kept track of such divergencies in our arguments, we nevertheless believe that they do not invalidate our main inequality (19) as further slow modes not captured by exact conservation laws will only increase the conductivity. It is, however, likely that the equality (21) is not valid for such situations. In Appendix C we analyze in some detail within the Boltzmann equation formalism under which conditions (21) holds. As an aside, we note that the singular heat transport of non-interacting disordered phonons, mentioned above, is well described within our formalism if we model the clean system by $H_0$ and the disorder by $H_1$, see the extensive discussion by Ziman within the variational approach which can be directly translated to the memory matrix language, see Ref. [26].

It would be interesting to generalize our results to cases where time reversal symmetry is broken, e.g. by an external magnetic field. As time reversal invariance entered nontrivially in our arguments, this seems not to be simple. We nevertheless do not see any physical reason why the inequality should not be valid in this case, too. One example where no problems arise are spin chains in a uniform magnetic field[31] where one can map the field to a chemical potential using a Jordan-Wigner transformation. Then one can directly apply our results to the time reversal invariant system of Jordan-Wigner fermions.

Acknowledgments

We thank N. Andrei, E. Shimshoni, P. Wölfle and X. Zotos for useful discussions. This work was partly supported by the Deutsche Forschungsgemeinschaft through SFB 608 and the German Israeli Foundation.

APPENDIX A: DRUDE WEIGHT AND MAZUR INEQUALITY

In this appendix we clarify the connection between the Drude weight and the Mazur inequality; mentioned in the introduction.

The Drude weight $D$ is the singular part of the conductivity at zero frequency, $\text{Re} \sigma(\omega) = \pi D \delta(\omega) + \sigma_{\text{reg}}(\omega)$. It can be calculated from the relation

$$D = \lim_{\omega \to 0} \omega \text{Im} \sigma(\omega).$$

It has been introduced by Kohn as a measure of ballistic transport, indicated by $D > 0$.

Using Kubo formulas, conductivities can be expressed in terms of the dynamic current susceptibilities $\Pi(z)$ using

$$\sigma(z) = -\frac{1}{iz} \left( \Pi^T - \Pi(z) \right),$$

where $\Pi(z)$ is the current response function

$$\Pi(z) = i \int_0^\infty dt e^{izt} \langle [J(t), J(0)] \rangle,$$

and $\Pi^T$ is a current susceptibility. The conductivity may be calculated by setting $\sigma(\omega) = \sigma(z = \omega + i0)$. Relation (A3) is a well known sum rule and for all regular correlation functions one has $\Pi^T = \Pi(0)$. In the presence of a singular contribution to $\sigma(\omega)$, one easily identifies the Drude weight with the expression $\Pi^T - \Pi(0)$. For this difference Mazur[32] derived a lower bound. Furthermore, Suzuki[33] has shown, that $\Pi^T - \Pi(0)$ may be expressed as a sum over all constants of the motion $C_i$ present in the system,

$$D = \Pi^T - \Pi(0) = \frac{1}{V} \sum_{n=0}^\infty \frac{\langle C_i J \rangle^2}{\langle C_i^2 \rangle},$$

Thus, the Drude weight is intimately connected to the presence of conservation laws: only components of the current perpendicular to all conservation laws decay and any conservation law with a component parallel to the current (i.e. with a finite cross-correlation $\langle C_i J \rangle$) leads to a finite Drude weight and thus ballistic transport. The relation between the Drude weight and Mazur’s inequality has been first pointed out by Zotos[34].

APPENDIX B: PERTURBATION THEORY FOR $1/\sigma$

Let us give an example of a naive perturbative derivation (see also Ref. [35]) to gain some insight about what problems can turn up in a perturbative derivation as the
one presented in this work. According to our assumptions, the conductivity is diverging for \( g \to 0 \) and therefore it is useful to consider the scattering rate \( \Gamma(\omega)/\chi \) (with the current susceptibility \( \chi \)) defined by

\[
\sigma(\omega) = \frac{\chi}{\Gamma(\omega)/\chi - i\omega}.
\] (B1)

If \( J \) is conserved for \( g = 0 \) (i.e. for \( J = J_g \), see above), the scattering rate vanishes, \( \Gamma(\omega) = 0 \), for \( g = 0 \), which results in a finite Drude weight. A perturbation around this singular point results in a finite \( \Gamma(\omega) \). In the limit \( g \to 0 \) we can expand \( \Gamma(\omega) \) for any finite frequency \( \omega \) in \( \Gamma \) to obtain

\[
\omega^2 \text{Re} \sigma(\omega) = \text{Re} \Gamma(\omega) + \mathcal{O}(\Gamma^2/\omega).
\] (B2)

We can read this as an equation for the leading order contribution to \( \Gamma(\omega) \), which now is expressed through the Kubo formula for the conductivity. By partially integrating twice in time we can write \( \Gamma(\omega) = \Gamma(\omega) + \mathcal{O}(g^2) \) with

\[
\text{Re} \Gamma(\omega) = \text{Re} \frac{1}{\sqrt{2}} \int_0^\infty dte^{izt} \langle [\hat{J}(t), \hat{J}(0)] \rangle \big|_{z = \omega + it},
\] (B3)

where \( \hat{J} = i[H, J] = ig[H_1, J] \) is linear in \( g \) and therefore the expectation value \( \langle ... \rangle_0 \) can be evaluated with respect to \( H_0 \) (which may describe an interacting system). Thus we have expressed the scattering rate via a simple correlation function of the time derivative of the current.

To determine the dc conductivity it is interested in the limit \( \omega \to 0 \) and it is tempting to set \( \omega = 0 \) in Eq. (B3). We have, however, derived Eq. (B3) in the limit \( g \to 0 \) at finite \( \omega \) and not in the limit \( \omega \to 0 \) at finite \( g \). The series Eq. (B2) is well defined for finite \( \omega \neq 0 \) only and in the limit \( \omega \to 0 \) the series shows singularities to arbitrarily high orders in \( 1/\omega \).

At first sight this makes Eq. (B3) useless for calculating the dc conductivity. One of the main results of this paper is that, nevertheless, \( \Gamma(\omega = 0) \) can be used to obtain a lower bound to the dc conductivity

\[
\sigma(\omega = 0) \geq \frac{\chi^2}{\Gamma(0)} \text{ for } g \to 0.
\] (B4)

**APPENDIX C: SINGLE SLOW MODE**

In this appendix we check whether in the presence of a single conservation law with finite cross correlations with the current the inequality (10) can be replaced by the equality (21). This requires us to compare the true conductivity, which in general is hard to determine, to the result given by \( \hat{M}_1 \). Thus we restrict ourselves to the discussion of models for which a Boltzmann equation can be formulated and the expression for the conductivity can be calculated at least numerically. In the following we first show numerically that the equality (21) holds for a realistic model. In a second step we discuss the precise regularity requirement of the scattering matrix such that Eq. (21) holds.

To simplify numerics, we consider a simple one-dimensional Boltzmann equation of interacting and weakly disordered Fermions. Clearly, the Boltzmann approach breaks down close to the Fermi surface due to singularities associated with the formation of a Luttinger liquid, but in the present context we are not interested in this physics as we only want to investigate properties of the Boltzmann equation. To avoid the restrictions associated with momentum and energy conservation in one dimension we consider a dispersion with two minima and four Fermi points,

\[
\epsilon_k = \frac{k^2}{2} + \frac{k^4}{4} + \frac{1}{10}.
\] (C1)

The Boltzmann equation reads

\[
v_k \frac{d f_k}{d t} = \sum_{k'qf} S_{kk'}^{qq'} [f_k f_{k'} (1 - f_q)(1 - f_{q'}) - f_q f_{q'} (1 - f_k)(1 - f_{k'})] + g^2 \sum_{k'} \delta (\epsilon_k - \epsilon_{k'}) [f_k (1 - f_{k'}) - f_{k'} (1 - f_k)]
\]

\[
= \sum_{k'} W_{kk'} \Phi_{k'}
\] (C2)

where the inelastic scattering term \( S_{kk'}^{qq'} = \delta (\epsilon_k + \epsilon_{k'} - \epsilon_q - \epsilon_{q'}) \delta (k + k' - q - q') \) conserves both energy and momentum. In the last line we have linearized the right hand side using the definitions of the introductory chapter. The velocity \( v_k \) is given by \( v_k = \frac{d}{dk} \epsilon_k \). The scattering matrix splits up into an interaction component and a disorder component, \( W_{kk'} \). As we do not consider Umklapp scattering, \( W_{kk'} \) conserves momentum, \( \sum_{k'} W_{kk'} k' = 0 \), and one expects that momentum relaxation will determine the conductivity for small \( g \).

For the numerical calculation we discretize momentum in the interval \([-\pi/2, \pi/2] \), \( k_n = n \delta k = n \pi/N \) with integer \( n \). (At the boundaries the energy is already too high to play any role in transport.) The delta function arising from energy conservation is replaced by a gaussian of width \( \delta \). The proper thermodynamic limit can for example be obtained by choosing \( \delta = 0.3 / \sqrt{N} \). The numerics shows small finite size effects.

In Fig. 2 we compare the numerical solution of the Boltzmann equation to the single mode memory matrix calculation or, equivalently, to the variational bound obtained by setting \( \Phi_k = k \) in Eq. (2)

\[
\tilde{\sigma} = \frac{\left( \sum_k v_k^2 k W_{kk'} \frac{g}{\delta k} \right)^2}{\left( \sum_{k,k'} k W_{kk'} k' \right)^2} = \frac{\left( \sum_k v_k^2 k W_{kk'} \frac{g}{\delta k} \right)^2}{g^2 \left( \sum_{k,k'} k W_{kk'} k' \right)^2}.
\] (C3)

As can be seen from the inset, in the limit of small \( g \) one obtains the exact value for the conductivity, which is what we intended to demonstrate.
Next we turn to an analysis of regularity conditions which have to be met in general by the scattering matrix $W_{kk'}$ such that convergence is guaranteed in the limit $g \to 0$. According to the assumptions of this appendix, for $g = 0$ the variational form of the Boltzmann equation (2) has a unique solution $\Phi = \bar{\Phi} + \Phi$ (i.e. $\sum_k \Phi_k \Phi_k^\dagger df^0/\partial \epsilon_k = 0$ and $\sum_k v_k \Phi_k df^0/\partial \epsilon_k > 0$).

In the presence of a finite, but small $g$ we write the solution of the Boltzmann equation as $\Phi = \bar{\Phi} + \Phi$, where $\Phi$ has no component parallel to $\bar{\Phi}$ (i.e. $\sum_k \Phi_k \Phi_k^\dagger df^0/\partial \epsilon_k = 0$). On the basis of the two inequalities

$$F[\Phi] \leq F[\bar{\Phi}]$$
$$\Phi W \Phi = \bar{\Phi} g^2 W^1 \bar{\Phi} + \Phi \perp W \Phi \perp \geq \bar{\Phi} g^2 W^1 \bar{\Phi}$$

one concludes that Eq. (21) is valid, i.e. that

$$\lim_{g \to 0} F[\Phi] = 1$$

under the condition that

$$\lim_{g \to 0} \sum_k v_k \Phi_k \frac{df^0}{\partial \epsilon_k} = \sum_k v_k \bar{\Phi}_k \frac{df^0}{\partial \epsilon_k}$$

or, equivalently,

$$\lim_{g \to 0} \sum_k v_k \Phi_{\perp,k} \frac{df^0}{\partial \epsilon_k} = 0. \quad (C6)$$

We therefore have to check whether $\Phi_{\perp}$ becomes small in the limit of small $g$.

Expanding the saddlepoint equation for (2) we obtain

$$\sum_{k'} W_{kk'}^0 \bar{\Phi}_{k'}^\dagger = v_k \frac{df^0}{\partial \epsilon_k} \sum_{k,k'} W_{kk'}^0 \bar{\Phi}_{k'}^\dagger \bar{\Phi}_{k'}^\perp + O(g^2 W^1_{kk'} \bar{\Phi}_{k'})$$

As by definition $\Phi^\perp$ has no component parallel to $\bar{\Phi}$, we can insert the projector $Q$ which projects out the conservation law in front of $\Phi^\perp$ on the left hand side. We therefore conclude that if the inverse of $W^0 Q$ exists, then $\Phi_{\perp}$ is of order $g^2$, Eq. (C6) is valid and therefore also Eq. (21). In our numerical examples these conditions are all met.

Under what conditions can one expect that Eq. (C6) is not valid? Within the assumptions of this appendix we have excluded the presence of other zero modes of $W^0$ (i.e. conservation laws) with finite overlap with the current. But it may happen that $W^0$ has many eigenvalues which are arbitrarily small such that the sum in Eq. (C6) diverges. In such a situation the presence of slow modes which cannot be identified with conservation laws of the unperturbed system invalidates Eq. (21).

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34 As $\Theta^2 = \pm 1$ for states with integer or half-integer spin, the combinations $A \Theta^\pm$ have signatures $\pm 1$ provided the operator $A$ does not change the total spin by half an integer, which is the case for all operators with finite cross-correlation functions with the physical currents.
35 The $C_i$ span the space of all conservation laws, including those which do not commute with each other.
36 More precisely, $\{C_i\}$ is taken to be a basis of the space of operators with energy-diagonal entries only, chosen to be orthogonal in the sense that $\langle C_i C_j \rangle \propto \delta_{ij}$.