Lower bounds for the conductivities of correlated quantum systems

Peter Jung and Achim Rosch
Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany
(Received 12 April 2007; published 7 June 2007)

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.

DOI: 10.1103/PhysRevB.75.245104 PACS number(s): 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 quasiparticles 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 noninteracting 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 noninteracting 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.[1–6]

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.[7]

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.[8] The linearized Boltzmann equation in the presence of a static electric field can be written in the form

$$e\mathbf{E}\mathbf{v}_{\mathbf{k}}\frac{df^0}{d\epsilon_{\mathbf{k}}}=\sum_{\mathbf{k}'}W_{\mathbf{k},\mathbf{k}'}\Phi_{\mathbf{k}'},\tag{1}$$

where $W_{\mathbf{k},\mathbf{k}'}$ is the integral kernel describing the scattering of quasiparticles, and we have linearized the Boltzmann equation around the Fermi (or Bose) distribution $f^0_{\mathbf{k}}=f^0(\epsilon_{\mathbf{k}})$ using $f_{\mathbf{k}}=f^0_{\mathbf{k}}-\frac{df^0}{d\epsilon_{\mathbf{k}}}\Phi_{\mathbf{k}}$. Therefore, the current is given by $\mathbf{I}=-e\Sigma_{\mathbf{k}}\mathbf{v}_{\mathbf{k}}\frac{df^0}{d\epsilon_{\mathbf{k}}}\Phi_{\mathbf{k}}$ and the dc conductivity is determined from the inverse of the scattering matrix W using $\sigma=-e^2\Sigma_{\mathbf{k}\mathbf{k}'}\frac{df^0}{d\epsilon_{\mathbf{k}}}v^i_{\mathbf{k}}W^{-1}_{\mathbf{k},\mathbf{k}'}v^i_{\mathbf{k}'}\frac{df^0}{d\epsilon_{\mathbf{k}'}}$. It is easy to see that this result can be obtained by maximizing a functional[8–11] $F[\Phi]$ with

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

$$F[\Phi]=\frac{2\left(\sum_{\mathbf{k}}v^i_{\mathbf{k}}\Phi_{\mathbf{k}}\frac{df^0}{d\epsilon_{\mathbf{k}}}\right)^2}{\sum_{\mathbf{k},\mathbf{k}'}(\Phi_{\mathbf{k}}-\Phi_{\mathbf{k}'})^2W_{\mathbf{k},\mathbf{k}'}},\tag{2}$$

where we used $\Sigma_{\mathbf{k}'}W_{\mathbf{k},\mathbf{k}'}=0$, reflecting the conservation of probability. The variational formula (2) is actually closely related[8] 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 Φ 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[8]).

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. Mazur[12] and later Suzuki[13] 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

$$\mathrm{Re}\,\sigma(\omega,T)=\pi D(T)\delta(\omega)+\sigma_{\mathrm{reg}}(\omega,T).\tag{3}$$

Such a Drude weight can arise only in the presence of exact conservation laws C_j with $[H,C_j]=0$. Suzuki[13] showed that

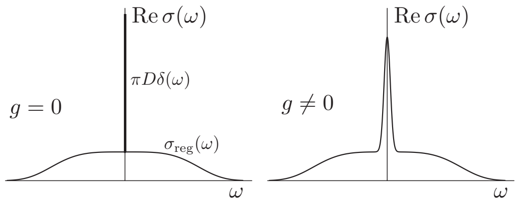

FIG. 1. For $g=0$, a Drude peak shows up in the conductivity, resulting from exact conservation laws. For $g\neq 0$, the Drude peak broadens and the dc conductivity becomes finite.

the Drude weight can be expressed as a sum over *all* C_j

$$D=\frac{\beta}{V}\sum_{j=0}^{\infty}\frac{\langle C_jJ\rangle^2}{\langle C_j^2\rangle}\geqslant\frac{\beta}{V}\sum_{j=0}^{N}\frac{\langle C_jJ\rangle^2}{\langle C_j^2\rangle},\tag{4}$$

where J is the current associated with σ. For convenience, a basis in the space of C_i has been chosen such that $\langle C_iC_j\rangle=0$ for $i\neq j$. More useful than the equality in Eq. (4) is often the inequality[12] 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[4,14–17] 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, interchain, disorder, phonon, etc.) renders the conductivity finite[1,4–6,18–20] If these perturbations are weak, the heat conductivity is, however, large as experimentally observed.[21,22] 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

$$H=H_0+gH_1,\tag{5}$$

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 noninteracting system. The term gH_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 quasiparticles. For technical reasons, 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 σ, which is the response of the current to some external field E coupling to the current,

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

where $J=\int j(x)$ is the total current and $\langle J\rangle$ its expectation value. Note that J can be an electrical, 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, $\langle JC_1\rangle\neq 0$. Without loss of generality, we assume $\langle C_iC_j\rangle=0$ for $i\neq j$. For $g=0$, the Drude weight D defined by Eq. (3) 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,

$$J=J_{\parallel}+J_{\perp},$$

with $J_{\parallel}=\Sigma_i\frac{\langle C_iJ\rangle}{\langle C_i^2\rangle}C_i$, which results in a separation of the conductivity,

$$\sigma(z)=\sigma_{\parallel}(z)+\sigma_{\perp}(z).\tag{6}$$

Since the conductivity $\sigma(z)$ is given by a current-current correlation function and the current $J_{\parallel}$ ($J_{\perp}$) is diagonal (off-diagonal) in energy, cross-correlation functions $\langle\langle J_{\parallel};J_{\perp}\rangle\rangle$ vanish in Eq. (6).

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

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

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

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 Sec. IV) 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 perturbed systems. 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,[23] introduced by Mori[24] and Zwanzig[25] 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,

$$(A|B) = \int_0^\beta d\lambda \langle A^\dagger B(i\lambda)\rangle - \beta\langle A^\dagger\rangle\langle B\rangle. \tag{8}$$

As the next step, we choose—for the moment—an 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,

$$(C_i|C_j) = \delta_{ij}. \tag{9}$$

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

$$P = \sum_i |C_i)(C_i| = 1 - Q.$$

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

$$|J) \equiv |C_1).$$

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 $|A(t))=|e^{iHt}Ae^{-iHt})=e^{iLt}|A)$. 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[23–25] that the conductivity can be expressed as the (1,1) component of the inverse of a matrix

$$\sigma(\omega) = (M(\omega) + iK - i\omega)^{-1}_{11}, \tag{10}$$

where

$$M_{ij}(\omega) = \left(\dot{C}_i\left|Q\frac{i}{\omega - LQ}\right|\dot{C}_j\right) \tag{11}$$

is the so-called memory matrix and

$$K_{ij} = (\dot{C}_i|C_j) \tag{12}$$

a frequency independent matrix. The formal expression (10) 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 (11) 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

$$[M(0) + K]^{-1}. \tag{13}$$

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[34] Θ. 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 $(C_m|\dot{C}_n)=0$, and thus, K vanishes on this restricted space. The dc conductivity therefore takes the form

$$\sigma = (M(0)^{-1})_{11}. \tag{14}$$

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 $\dot{C}_i = ig[H_1, C_i]$ 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., the Drude peak appearing in Eq. (3) is the only singular contribution. Furthermore, we choose $J=J_\parallel=C_1$ 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 $(.|.)$ with $(.|.)_0$ as we evaluate the scalar product with respect to H_0. As $L_0|C_i)=0$ and $(C_j|\dot{C}_i)=0$ due to time reversal symmetry, one has $L_0Q=1$ and $Q|\dot{C}_i)=|\dot{C}_i)$, and therefore, the projector Q does not contribute within this approximation. We, thus, define the $n\times n$ matrix $\tilde{M}_n$ by

$$\tilde{M}_{n,ij} = \lim_{\omega\to 0}\left(\dot{C}_i \left| \frac{i}{\omega - L_0} \right| \dot{C}_j\right)_0. \tag{15}$$

Note that $\tilde{M}_n$ is a submatrix of $\tilde{M}_m$ for $m > n$, and therefore, the approximate expression for the conductivity $\sigma \approx (\tilde{M}_n^{-1})_{11}$ does depend on n while $(M_n^{-1})_{11}$ 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,

$$\sigma|_{1/g^2} = (\tilde{M}_\infty^{-1})_{11} \geq \cdots \geq (\tilde{M}_n^{-1})_{11} \geq \cdots \geq \tilde{M}_1^{-1}. \tag{16}$$

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 σ. Note that $\tilde{M}_n \propto g^2$ by construction. $\tilde{M}_\infty$ is the approximate memory matrix, where *all*[35] 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. (B4) in Appendix B, as the scattering rate $\tilde{\Gamma}/\chi$ may be expressed as $\tilde{\Gamma}/\chi^2 = \tilde{M}_1$.

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 $\tilde{M}_n$ 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 Eq. (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 $\tilde{M}_{n<\infty}$). This, in turn, implies that $\lim_{g\to 0} M_\infty/g^2 = \tilde{M}_\infty/g^2$, and therefore, $\sigma|_{1/g^2} = (\tilde{M}_\infty^{-1})_{11}$.

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

$$(\tilde{M}_\infty^{-1})_{11} = \max_{\boldsymbol{\varphi}} \frac{(\boldsymbol{\varphi}^T \boldsymbol{e}_1)^2}{\boldsymbol{\varphi}^T \tilde{M}_\infty \boldsymbol{\varphi}}, \tag{17}$$

where $\boldsymbol{e}_1$ 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 $\boldsymbol{\varphi} = \tilde{M}_\infty^{-1}\boldsymbol{e}_1$. By restricting the variational space in Eq. (17) to the first n components of $\boldsymbol{\varphi}$, we reproduce the submatrix $\tilde{M}_n$ of $\tilde{M}_\infty$ and obtain

$$(\tilde{M}_\infty^{-1})_{11} \geq \max_{\boldsymbol{\varphi}=\sum_1^m \varphi_i e_i} \frac{(\boldsymbol{\varphi}^T e_1)^2}{\boldsymbol{\varphi}^T \tilde{M}_\infty \boldsymbol{\varphi}} = (\tilde{M}_m^{-1})_{11} \geq \max_{\boldsymbol{\varphi}=\sum_1^{n<m} \varphi_i e_i} \frac{(\boldsymbol{\varphi}^T e_1)^2}{\boldsymbol{\varphi}^T \tilde{M}_\infty \boldsymbol{\varphi}}$$

$$= (\tilde{M}_{n<m}^{-1})_{11}.$$

By choosing different values for m and $n < m$, this proves all inequalities appearing in Eq. (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 $LQ_n = L_0 + gL_1Q_n$, we obtain the geometric series

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

Note that this is not a full expansion in g, as the scalar product (8) is defined with respect to the full Hamiltonian $H = H_0 + gH_1$. We will turn to the discussion of the remaining g dependence later.

In general, one can expand

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

in terms of some basis A_m in the space of operators. Therefore, Eq. (18) can be written as a sum over products of terms with the general structure

$$\left(A \left| Q_n \frac{1}{\omega - L_0} \right| B\right). \tag{19}$$

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_∞ 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_∞ is regular.

To show this more formally, we split up $B = B_\parallel + B_\perp$ in Eq. (19) into a component parallel and one perpendicular to the space of all conserved quantities, $|B_\parallel) = P_\infty |B)$. With this notation, the action of L_0 becomes more transparent:

$$\frac{1}{\omega - L_0}|B) = \frac{1}{\omega}|B_\parallel) + \frac{1}{\omega - L_0}|B_\perp). \tag{20}$$

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 $(A|Q_n|B_\parallel)$ 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 $(A|Q_n|B_\parallel)$ exist and the perturbative series in g will be singular (see also Appendix B). Considering M_∞, however, Q_∞ projects out all conservation laws, and therefore, by construction $Q_\infty|B_\parallel)=Q_\infty P_\infty|B)=0$. Thus, the first term in Eq. (20) does not contribute in Eq. (19) for $n=\infty$ and the expansion (18) of M_∞ is therefore regular.

The only remaining part of our argument is to show that in the limit $g\to 0$ one can safely replace $(.|.)$ with $(.|.)_0$. Here, it is useful to realize that $(A|B)$ can be interpreted as a (generalized) static susceptibility. In the absence of a phase transition and at finite temperatures, susceptibilities are smooth, nonsingular 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 susceptibilities 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 $(\dot{C}_i|Q_\infty=(\dot{C}_i|$ [see discussion before Eq. (15)], its leading term, $k=0$, is given by $\tilde{M}_\infty$. 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 σ without further complications.

The relevant lower bounds are directly obtained from the memory matrix formalism. Typically,[26–28] 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 noninteracting system.[26] For situations where the Boltzmann equation can be applied, it has been pointed out a long time ago by Belitz[29] 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 noninteracting bosonic system, then typical perturbations are of the form cos ϕ, 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 model[6] or some nontrivial quantum-field theory.[30] In these cases, it can become difficult to calculate the memory matrix and one has to resort to using either numerical[6] or field-theoretical methods[30] 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 nontrivial 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 $\tilde{M}_\infty=\tilde{M}_1$ in this case, our results suggest that for small g the conductivity is *exactly* determined by the momentum relaxation rate $\tilde{M}_{PP}=\lim_{\omega\to 0} i(\dot{P}|(\omega-L_0)^{-1}|\dot{P})$,

$$\sigma = \frac{\chi_{PJ}^2}{\tilde{M}_{PP}} \quad \text{for } g\to 0. \tag{21}$$

Here we used $J_\parallel = P(P|J)/(P|P)$ with $\chi_{PJ}=(P|J)$ and we have restored all factors which arise if the normalization condition (9) is not used. In Appendix C, we numerically check 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., noninteracting phonons in a disordered crystal[8]). 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 (16) 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 Eq. (21) holds. As an aside, we note that the singular heat transport of noninteracting 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[8] within the variational approach, which can be directly translated to the memory matrix language; see Ref. 29).

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 Sec. I

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

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

It has been introduced by Kohn[32] as a measure of ballistic transport, indicated by $D>0$.

Using Kubo formulas, conductivities can be expressed in terms of the dynamic current susceptibilities[33] $\Pi(z)$ using

$$\sigma(z)=-\frac{1}{iz}(\Pi^T-\Pi(z)), \tag{A1}$$

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

$$\Pi(z)=\frac{i}{V}\int_0^\infty dt e^{izt}\langle[J(t),J(0)]\rangle, \tag{A2}$$

$$\Pi^T=\int\frac{d\omega}{\pi}\frac{\Pi''(\omega)}{\omega}, \tag{A3}$$

and Π^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[12,13] derived a lower bound. Furthermore, Suzuki[13] 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,[36]

$$D=\Pi^T-\Pi(0)=\frac{\beta}{V}\sum_{n=0}^{\infty}\frac{\langle C_jJ\rangle^2}{\langle C_j^2\rangle}. \tag{A4}$$

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 $\langle C_jJ\rangle$) 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 *et al.*[14]

APPENDIX B: PERTURBATION THEORY FOR 1/σ

Let us give an example of a naive perturbative derivation (see also Ref. 6) 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 χ) defined by

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

If J is conserved for $g=0$ (i.e., for $J=J_\parallel$, see above), the scattering rate vanishes, $\Gamma(\omega)=0$, 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 Eq. (B1) for any *finite* frequency ω in Γ to obtain

$$\omega^2\,\mathrm{Re}\,\sigma(\omega)=\mathrm{Re}\,\Gamma(\omega)+\mathcal{O}(\Gamma^2/\omega). \tag{B2}$$

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 $\Gamma(\omega)=\tilde{\Gamma}(\omega)+\mathcal{O}(g^3)$ with

$$\mathrm{Re}\,\tilde{\Gamma}(\omega)=\mathrm{Re}\,\frac{1}{z}\frac{1}{V}\int_0^\infty dt e^{izt}\langle[\dot{J}(t),\dot{J}(0)]\rangle_0\Big|_{z=\omega+i0}, \tag{B3}$$

where $\dot{J}=i[H,J]=ig[H_1,J]$ is linear in g, and therefore, the expectation value $\langle\cdots\rangle_0$ 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, one 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 ω 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, $\tilde{\Gamma}(\omega=0)$ can be used to obtain a lower bound to the dc conductivity

$$\sigma(\omega=0)\geq\frac{\chi^2}{\tilde{\Gamma}(0)}\quad\text{for } g\to 0. \tag{B4}$$

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 (16) can be replaced with the equality (21). This requires us to compare the true conductivity, which, in general, is hard to determine, to the result given by $\tilde{M}_1$. 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,

$$\epsilon_k = -\frac{k^2}{2} + \frac{k^4}{4} + \frac{1}{10}. \tag{C1}$$

The Boltzmann equation reads

$$v_k \frac{df_k^0}{d\epsilon_k} E = \sum_{k' q q'} S_{kk'}^{qq'} [f_k f_{k'} (1-f_q)(1-f_{q'}) - f_q f_{q'} (1-f_k) \times (1-f_{k'})] + g^2 \sum_{k'} \delta(\epsilon_k - \epsilon_{k'}) [f_k (1-f_{k'}) - f_{k'} (1-f_k)] = \sum_{k'} W_{kk'} \Phi_{k'}, \tag{C2}$$

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 Sec. I. 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, $W_{kk'} = W_{kk'}^0 + g^2 W_{kk'}^1$. As we do not consider umklapp scattering, $W_{kk'}^0$ conserves momentum, $\Sigma_{k'} W_{kk'}^0 k' = 0$, 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 δ. 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,[29] to the variational bound obtained by setting $\Phi_k = k$ in Eq. (2),

$$\tilde{\sigma} = \frac{\left(\sum_k v_k^i k \frac{df^0}{d\epsilon_k}\right)^2}{\sum_{k,k'} k W_{kk'} k'} = \frac{\left(\sum_k v_k^i k \frac{df^0}{d\epsilon_k}\right)^2}{g^2 \sum_{k,k'} k W_{kk'}^1 k'}. \tag{C3}$$

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.

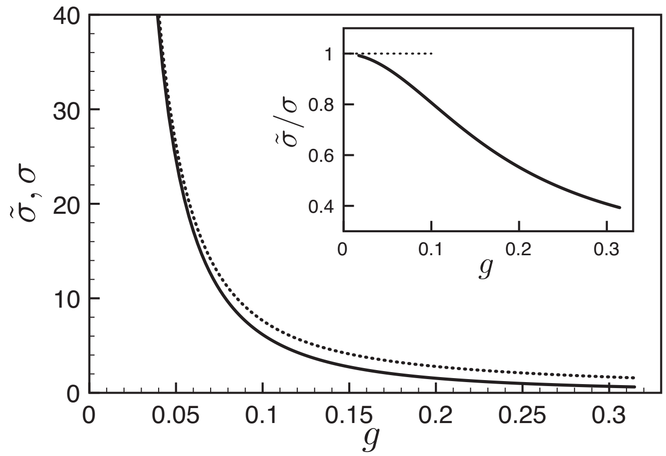

FIG. 2. Comparison of the result of a single mode memory matrix calculation (solid line) [Eq. (C3)] to the full numerical solution of the Boltzmann equation (dotted line) for $T=0.05$ and $N=500$. The memory matrix is always a lower bound to the Boltzmann result and converges toward it as the disorder strength g is reduced, as shown in the inset (ratio of the single mode approximation to the Boltzmann result).

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 $\bar{\Phi}_k$ (up to a multiplicative constant), with $F(\bar{\Phi}_k) = \infty$, $\Sigma_{k'} W_{kk'}^0 \bar{\Phi}_{k'} = 0$ and $\Sigma_k v_k \bar{\Phi}_k df^0/d\epsilon_k > 0$.

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

$$F[\bar{\Phi}] \leq F[\Phi], \tag{C4}$$

$$\Phi W \Phi = \bar{\Phi} g^2 W^1 \bar{\Phi} + \Phi_{\perp} W \Phi_{\perp} \geq \bar{\Phi} g^2 W^1 \bar{\Phi}, \tag{C5}$$

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

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

under the condition that

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

or, equivalently,

$$\lim_{g\to 0} \sum_k v_k \Phi_{\perp,k} \frac{df^0}{d\epsilon_k} = 0. \tag{C6}$$

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

Expanding the saddle point equation for Eq. (2), we obtain

$$\sum_{k'} W^0_{kk'}\Phi^{\perp}_{k'} = v_k \frac{df^0}{d\epsilon_k} \frac{\sum_{k'k''} \bar{\Phi}_{k'} g^2 W^1_{k'k''} \bar{\Phi}_{k''}}{\sum_{k'} v_{k'} \frac{df^0}{d\epsilon_{k'}} \bar{\Phi}_{k'}} - \sum_{k'} g^2 W^1_{kk'} \bar{\Phi}_{k'} + \mathcal{O}(g^2 W_1 \Phi_{\perp}, \Phi_{\perp} W_0 \Phi_{\perp}).$$

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 $\Phi^{\perp}_k$, 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. However, 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).

[1] X. Zotos and P. Prelovsek, Phys. Rev. B **53**, 983 (1996).
[2] K. Fabricius and B. M. McCoy, Phys. Rev. B **57**, 8340 (1998).
[3] B. N. Narozhny, A. J. Millis, and N. Andrei, Phys. Rev. B **58**, R2921 (1998).
[4] X. Zotos and P. Prelovsek, *Interacting Electrons in Low Dimensions*, Physics and Chemistry of Materials with Low-Dimensional Structures (Kluwer Academic, Dordrecht, in press).
[5] F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Physica B **359**, 1394 (2005).
[6] P. Jung, R. W. Helmes, and A. Rosch, Phys. Rev. Lett. **96**, 067202 (2006).
[7] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[8] J. Ziman, *Electrons and Phonons: The Theory of Transport Phenomena in Solids* (Oxford University Press, New York, 1960).
[9] M. Kohler, Z. Phys. **124**, 772 (1948).
[10] M. Kohler, Z. Phys. **125**, 679 (1949).
[11] E. H. Sondheimer, Proc. R. Soc. London, Ser. A **203**, 75 (1950).
[12] P. Mazur, Physica (Amsterdam) **43**, 533 (1969).
[13] M. Suzuki, Physica (Amsterdam) **51**, 277 (1971).
[14] X. Zotos, F. Naef, and P. Prelovsek, Phys. Rev. B **55**, 11029 (1997).
[15] S. Fujimoto and N. Kawakami, Phys. Rev. Lett. **90**, 197202 (2003).
[16] F. Heidrich-Meisner, A. Honecker, and W. Brenig, Phys. Rev. B **71**, 184415 (2005).
[17] K. Sakai, Physica E (Amsterdam) **29**, 664 (2005).
[18] E. Shimshoni, N. Andrei, and A. Rosch, Phys. Rev. B **68**, 104401 (2003).
[19] F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, Phys. Rev. B **66**, 140406(R) (2002).
[20] A. V. Rozhkov and A. L. Chernyshev, Phys. Rev. Lett. **94**, 087201 (2005).
[21] A. V. Sologubenko, E. Felder, K. Giannò, H. R. Ott, A. Vietkine, and A. Revcolevschi, Phys. Rev. B **62**, R6108 (2000).
[22] C. Hess, H. El Haes, A. Waske, B. Buchner, C. Sekar, G. Krabbes, F. Heidrich-Meisner, and W. Brenig, Phys. Rev. Lett. **98**, 027201 (2007).
[23] *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions*, edited by D. Forster (Perseus, New York, 1975).
[24] H. Mori, Prog. Theor. Phys. **33**, 423 (1965).
[25] R. Zwanzig, in *Lectures in Theoretical Physics*, edited by W. E. Brittin, B. W. Downs, and J. Downs (Interscience, New York, 1961), Vol. III; J. Chem. Phys. **33**, 1338 (1960).
[26] W. Götze and P. Wölfle, Phys. Rev. B **6**, 1226 (1972).
[27] T. Giamarchi, Phys. Rev. B **44**, 2905 (1991).
[28] A. Rosch and N. Andrei, Phys. Rev. Lett. **85**, 1092 (2000).
[29] D. Belitz, J. Phys. C **17**, 2735 (1984).
[30] E. Boulat, P. Mehta, N. Andrei, E. Shimshoni, and A. Rosch, e-print arXiv:cond-mat/0607837.
[31] A. V. Sologubenko, K. Berggold, T. Lorenz, A. Rosch, E. Shimshoni, M. D. Phillips, and M. M. Turnbull, Phys. Rev. Lett. **98**, 107201 (2007).
[32] W. Kohn, Phys. Rev. **133**, 171 (1964).
[33] L. P. Kadanoff and P. C. Martin, Ann. Phys. (N.Y.) **24**, 419 (1963).

[34] As $\Theta^2 = \pm 1$ for states with integer or half-integer spin, the combinations $A \pm \Theta A \Theta^{-1}$ have signatures ± 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 $\langle C_i C_j \rangle \propto \delta_{ij}$.