New formulation of the Kubo Optical Conductivity: a Shortcut to Transport Properties

G. De Filippis\textsuperscript{1}, V. Cataudella\textsuperscript{1}, A. de Cандia \textsuperscript{1}, A. S. Mishchenko\textsuperscript{2} and N. Nagaosa\textsuperscript{2,3}

\textsuperscript{1}SPIN-CNR and Dip. di Fisica - Università di Napoli Federico II - I-80126 Napoli, Italy
\textsuperscript{2}RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan
\textsuperscript{3}Department of Applied Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

The Kubo formula for the electrical conductivity is rewritten in terms of a sum of Drude-like contributions associated to the exact eigenstates of the interacting system, each characterized by its own frequency-dependent relaxation time. The structure of the novel and equivalent formulation, weighting the contribution from each eigenstate by its Boltzmann occupation factor, simplifies considerably the access to the static properties (dc conductivity) and resolves the long standing difficulties to recover the Boltzmann result for dc conductivity from the Kubo formula. It is shown that the Boltzmann result, containing the correct transport scattering time instead of the electron lifetime determined by the Green function, can be recovered in problems with elastic and inelastic scattering at the lowest order of interaction.

PACS numbers: 72.10.-d, 72.10.Bg, 71.38.-k

INTRODUCTION

The electrical resistivity of a metal coming from the scattering with phonons or impurities is an important topic in the condensed matter physics and it has been addressed by using a large number of theoretical methods\textsuperscript{1-3}. In particular, one of the most powerful tool for investigating the metal transport properties is represented by the Boltzmann equation\textsuperscript{1,2}. It is derived on the basis of phenomenological assumptions within a semiclassical approach, and it is mostly suitable for the calculation of the electrical resistivity in the often encountered weak coupling regime. Indeed, by indicating with $\lambda$ a dimensionless parameter characterizing the strength of the coupling with phonon or impurities, even in the weak coupling limit, contrary to many physical properties, the analysis of the dc conductivity, $\sigma_{dc}$, is not a trivial problem since $\sigma_{dc}$ displays a singularity at $\lambda = 0$, i.e. $\sigma_{dc} \rightarrow \infty$ when $\lambda \rightarrow 0$. In particular $\sigma_{dc}$ can be expanded in a Laurent series in $\lambda$, near $\lambda = 0$, with the lowest order term of the order of $\lambda^{-2}$. Although very good for the description of the transport properties at small values of $\lambda$, the Boltzmann approach can not be systematically extended to any coupling and finite frequencies. On the other hand, the dynamic charge response to an electric field can be derived by using the quantum linear response theory and the Kubo formula\textsuperscript{3-5} whose validity is not restricted to the weak coupling regime. However, in the standard Kubo formulation (SKF), it is not straightforward to extract the leading term in the weak coupling limit since low-frequency divergences appear. Two remedies to this problem have been proposed in literature. One is the van Hove’s $\lambda^2 t$ limit\textsuperscript{6-8}, where if the limits $\lambda \rightarrow 0$ and $t \rightarrow \infty$ ($t$ is the time) with $\lambda^2 t = \text{const}$ are performed, one gets an expansion of the dc conductivity where each term is finite. However, the ad hoc recipe to fix $\lambda^2 t$ is not justified. The other proposal proceeds by expressing the response function in terms of a self-energy. It is based on the projection technique introduced by Mori\textsuperscript{9} and Zwanzig\textsuperscript{10} and the memory function formalism\textsuperscript{10,11}. In the following we will call it standard formulation of the optical conductivity (SFOC). In this approach, to circumvent the divergence of $\sigma_{dc}$, the idea is to expand $1/\sigma_{dc}$ in successive powers of $\lambda$. Evaluation of the memory function at the lowest order of $\lambda$ gives the classical Drude formula $\sigma_{dc} = ne^2\tau/m$ which, however, contains a relaxation time different from that entering into the Boltzmann solution\textsuperscript{12}. The last flaw can be fixed, though it requires a trick similar to the joint $\lambda^2 t$ limit: within SFOC the correct weak coupling limit requires again partial summation of infinite series of contributions\textsuperscript{12}.

In this paper we derive a Boltzmann weighted formulation of the optical conductivity (BWFOC), which is equivalent to the Kubo formula\textsuperscript{3}, but that has significant advantages over both Boltzmann solution and SFOC. BWFOC trivially reproduces the Boltzmann approach results without any artificial conditions of joint limits and without the necessity of partial summations of infinite series of contributions. On the other hand BWFOC retains all advantages of SFOC, like the possibility to consider finite frequencies and to make a systematic improvement of the result in higher orders of the interaction $\lambda$.

KUBO FORMULA

The SKF provides the linear response to a small electric field, along $x$ axis, of a system in thermodynamic
equilibrium (units are such that \( \hbar = 1 \)):

\[
\sigma(z) = \frac{i}{zV} \langle \Pi(z) - q_e^2 \Gamma \rangle ,
\]

where \( V \) is the system volume, \( z \) lies in the complex upper half-plane, \( z = \omega + i\epsilon \) with \( \epsilon > 0 \), \( q_e \) is the electronic charge, the quantity \( \Gamma \), in absence of superconductivity and in the thermodynamic limit, is given by:

\[
q_e^2 \Gamma = - \int_0^\beta d\tau \langle J(\tau) J(0) \rangle ,
\]

and \( \Pi(z) \) is the current-current correlation function

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

In Eq. 3 (Eq. 2) \( J(t) \langle J(\tau) \rangle \) is the (imaginary time) Heisenberg representation of the current operator along the \( x \) axis, \( [\cdot, \cdot] \) denotes the commutator, and \( \langle \cdot \rangle \) indicates the thermodynamical average.

By choosing the eigenbasis of the interacting system Hamiltonian, it is straightforward to show\[15\] that the real part of the optical conductivity, after performing the limit \( \epsilon \rightarrow 0^+ \), can be written as

\[
\Re \sigma(\omega) = D \delta(\omega) + \sigma_{\text{reg}}(\omega),
\]

where the regular part \( \sigma_{\text{reg}}(\omega) \) is defined by:

\[
\sigma_{\text{reg}}(\omega) = \sum_{n,m} \sum_{\epsilon_m \neq \epsilon_n} \frac{\pi}{V} \frac{|\langle \psi_n | J | \psi_m \rangle|^2}{\omega_{nm}} \delta(\omega - \omega_{nm}) (p_n - p_m) .
\]

Above \( p_n = e^{-\beta \epsilon_n}/Z \) is the Boltzmann weight of the eigenstate \( | \psi_n \rangle \), \( \epsilon_n \) is the corresponding energy, \( Z \) is the partition function, \( \omega_{nm} = \epsilon_m - \epsilon_n \), \( \beta = 1/K_BT \), \( K_B \) being the Boltzmann constant, and the Drude weight \( D \), i.e. the coefficient of the zero frequency delta function contribution, is given by\[15\]

\[
D = \frac{\pi \beta}{V} \sum_{\epsilon_m = \epsilon_n} p_n \frac{|\langle \psi_n | J | \psi_m \rangle|^2}{\omega_{nm}} .
\]

\( \sigma(\omega) \) satisfies the sum rule\[14\]

\[
\int_{-\infty}^{\infty} d\omega \Re \sigma(\omega) = -\frac{\pi q_e^2 \Gamma}{V} .
\]

The SKF is the most frequently used formulation for the calculation of the quantum optical conductivity. However we note that in this formulation \( \Re \sigma(\omega) \) shows a singularity at \( \omega = 0 \) if one proceeds perturbatively. Indeed, at \( \lambda = 0 \), \( \sigma_{\text{reg}}(\omega) = 0 \) so that only the coefficient \( D \) turns to be nonzero. As consequence the evaluation of the current-current correlation function by an expansion in a small parameter fails due to the singular behavior at small frequencies.

**MEMORY FUNCTION FORMULATION**

To overcome the difficulties related to the diagrammatic techniques that have to deal with summing divergent series, the SFOM was suggested, where one represents \( \sigma(z) \) in terms of a memory function \( M(z) \)\[10,12\]:

\[
\sigma(z) = -\frac{i}{V} \frac{q_e^2 \Gamma}{z + iM(z)} ,
\]

with

\[
M(z) = \frac{z\Pi(z)}{\Pi(z) - q_e^2 \Gamma} .
\]

This approach, introduced earlier by Kadanoff and Martin\[17\], allows to extract easily the resonance structures of the optical absorption due to the relaxation processes, since the memory function \( M(z) \) has a simple expansion in the lowest order in the impurity concentration and the electron-phonon coupling\[10\]. Indeed, by taking into account that \( \Pi(z) \) decreases as \( 1/z^2 \) when \( z \rightarrow \infty \), the first step is to expand \( M(z) \) at high frequencies (short time expansion) so that \( M(z) \approx -i\Pi(z)/q_e^2 \Gamma \). Successively, by using the equations of motion of the Green functions, one can express the product \( z\Pi(z) \) in terms of the force-force correlation function \( F(z) \), a Green function, involving the commutator between the current operator and the Hamiltonian:

\[
z\Pi(z) = \frac{F(z) - F(z = 0)}{z} ,
\]

with

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

Weak coupling and low frequency limit of SFOC give the classical Drude formula but with a wrong relaxation time. The relaxation time in the Boltzmann expression is the average of the relaxation times related to the eigenstates of the system in absence of the interaction \( \tau_{\text{av}} \). On the other hand in SFOC it is \( (1/\tau_{\text{av}})^{-1} \), i.e. since SFOC approach, at the lowest order, averages the inverse relaxation times, recovery of the Boltzmann formula requires a procedure equivalent to the \( \lambda^2 t \) limit.

**NEW FORMULATION OF THE OPTICAL CONDUCTIVITY**

Here we derive the BWFOC, which overcomes the above described difficulties. We note that \( \Pi(z) \) is analytic in the upper half of the complex plane and vanishes as \( z \rightarrow \infty \). Consequently \( \Pi(z) \) can be represented as a spectral integral

\[
\Pi(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{3\Pi(\omega)}{\omega - z} .
\]
On the other hand $\Xi\Pi(\omega)$ can be expressed in terms of the Fourier transform of symmetrized correlation function $\langle (J(t)J(0) + J(0)J(t)) \rangle$:

$$\Psi(z) = -i \sum_{0}^{\infty} dte^{izt} \langle (J(t)J(0) + J(0)J(t)) \rangle,$$

i.e. $\Xi\Pi(\omega) = \text{tanh}(\beta\omega/2)\Psi(\omega)$. Successively, by introducing the Lehmann representation of the correlation function $\Xi\Psi(\omega)$, using the Eq. (11) and writing the quantity $\Gamma$ in the eigenbasis of the interacting system Hamiltonian, one obtains $\Gamma = \sum_{n} p_{n} (\gamma_{n} + \nu_{n})$ and $\Pi(z) = \sum_{n} p_{n} \Pi_{n}(z)$, where:

$$\gamma_{n} = -\sum_{\epsilon_{n} \neq \epsilon_{m}} \frac{2 |\langle \psi_{n} | J | \psi_{m} \rangle|^{2}}{q_{e}^{2}\omega_{nm}} \text{tanh} \left( \frac{\beta\omega_{nm}}{2} \right),$$

and

$$\nu_{n} = \frac{\beta}{q_{e}^{2}} \left( -\sum_{\epsilon_{n} = \epsilon_{m}} |\langle \psi_{n} | J | \psi_{m} \rangle|^{2} \right),$$

$$\Pi_{n}(z) = \sum_{\epsilon_{n} \neq \epsilon_{m}} \frac{2 \left| \langle \psi_{n} | J | \psi_{m} \rangle \right|^{2}}{q_{e}^{2}\epsilon_{m}^{2}} \text{tanh} \left( \frac{\beta\omega_{nm}}{2} \right) f_{nm}(z).$$

Here $f_{nm}(z) = \frac{1 - \text{tanh}(\beta\epsilon_{m}/2)}{1 - \text{tanh}(\beta\epsilon_{m}/2)}$. In terms of the microcanonical quantities $s_{n} = \gamma_{n} + \nu_{n}$ and $\Pi_{n}(z)$, the BWFOC reads

$$\sigma(z) = \sum_{n} p_{n} \sigma_{n}(z),$$

where

$$\sigma_{n}(z) = \frac{i}{zV} \left( \Pi_{n}(z) - q_{e}^{2}s_{n} \right).$$

One can introduce now, for each of the quantum numbers $n$ labelling the eigenstates of the Hamiltonian, separate relaxation or memory function $M_{n}(z)$ (see Appendix for proof)

$$\sigma_{n}(z) = -\frac{i q_{e}^{2}s_{n}}{zVz + iM_{n}(z)},$$

with

$$M_{n}(z) = i \frac{z\Pi_{n}(z)}{\Pi_{n}(z) - q_{e}^{2}s_{n}}.$$

Finally, by taking into account that $z f_{nm}(z) = \omega_{nm} f_{nm}(z)$, where $f_{nm}(z) = \frac{1}{1 + z + \omega_{nm}}$, one can express the product $z f_{n}(z)$ in terms of the commutator between the current and Hamiltonian operators:

$$f_{n}(z) = \sum_{\epsilon_{n} \neq \epsilon_{m}} \frac{\left| \langle \psi_{n} | J | \psi_{m} \rangle \right|^{2}}{\omega_{nm}} \text{tanh} \left( \frac{\beta\omega_{nm}}{2} \right) f_{nm}(z),$$

that is the analogous of the introduction of the force-force correlation function in the new formulation. The set of equations [15-20] represents the BWFOC.

The BWFOC restores the semiclassical Boltzmann result at the lowest order in the coupling strength but it allows also a non trivial generalization to all frequencies and couplings. Namely, in all Boltzmann-like treatments a similar formula can be derived but with frequency independent memory function $M_{n}(z) = 1/\tau_{n}$. Furthermore the quantities $s_{n}$, $\tau_{n}$, and $p_{n}$ are exact in BWFOC, whereas they are calculated in a perturbative way within the Boltzmann approach.

We also point out that SKF and SFOC result in general expressions involving only the response function which can be represented in any basis. On the other hand, the new formulation explicitly relies on the use of eigenstates as basis. This more limited choice allows to incorporate explicitly the Boltzmann weight.

In order to recover the Boltzmann result we decompose the full Hamiltonian $H$ as $H = H_{0} + V$, where $V$ is the interaction potential which gives rise to dissipation, and suppose that $V$ is momentum independent and that the solid is homogeneous. In this case the conductivity tensor reduces to just the diagonal terms and they are equal, so that $\sigma_{n}(z) = \sum_{l=1}^{d} \sigma_{n,l}(z)/d$, where $d$ is the system dimensionality and $l$ indicate the lattice axes directions. The Eq. (18) assumes the following form:

$$\sigma_{n}(z) = -\frac{i q_{e}^{2}s_{n}}{dVz + iM_{n}(z)},$$

where $s_{n} = \sum_{l=1}^{d} s_{n,l}$, $\Pi_{n}(z) = \sum_{l=1}^{d} \Pi_{n,l}(z)$, and $M_{n}(z) = iz\Pi_{n}(z)/\Pi_{n}(z) - q_{e}^{2}s_{n}$. By approximating the exact eigenstates and eigenvalues with that ones of $H_{0}$, noticing that the matrix elements of the current operator between eigenstates of $H_{0}$ associated to different eigenvalues are zero, putting $z = \epsilon i$ and performing the limit $\epsilon \to 0^{+}$, one obtains:

$$\sigma_{dc}^{(0)} = \frac{\beta}{dV} \sum_{n} p_{n}^{(0)} r_{n}^{(0)} \sum_{\epsilon_{m}^{(0)} = \epsilon_{m}^{(0)}}^{d} \left| \langle \psi_{n}^{(0)} | J_{l} | \psi_{m}^{(0)} \rangle \right|^{2},$$

where the relaxation time associated to the eigenstate of $H_{0}$ with eigenvalue $\epsilon_{n}^{(0)}$ is:

$$\frac{1}{\tau_{n}^{(0)}} = \pi \sum_{m,l=1}^{d} \left( \left| \langle \psi_{n}^{(0)} | J_{l} | \psi_{m}^{(0)} \rangle \right|^{2} \delta(\epsilon_{n}^{(0)} - \epsilon_{m}^{(0)}) \right).$$

$J_{l}$ being the component of the current operator along the l-direction. In the following we show that, on the basis of this new formula, some known results can be easily reproduced, but also that new results can be deduced in inelastic scattering problems.
SCATTERING BY IMPURITIES

As first example we consider a noninteracting electron gas scattered by spin-independent impurity potentials. In this case \( H_0 = \sum_k \epsilon_k c_k^\dagger c_k \) with \( \epsilon_k(0) = k^2/2m \) and \( J_l = q_e \sum_k \frac{k}{m} c_k^\dagger c_k \). Taking into account that \([J_l, H_0] = 0\) and that the eigenvectors of the non interacting Hamiltonian are labelled by the total wavenumber \( \vec{k} \), the matrix element \( \langle \vec{k} | [J_l, V] | \vec{k} \rangle \) provides: \( q_e (k_l - k_l') \left( \langle \vec{k} | V | \vec{k} \rangle \right) / m \). It is straightforward to show that the dc conductivity becomes:

\[
\sigma_{dc}^{(0)} = -\frac{q_e^2}{eV m^2} \sum_k f_k' k^2 \tau_k^{(0)},
\]

with \( \frac{1}{\tau_k^{(0)}} = 2 \pi \sum_{\vec{k}'} \left| V_{\vec{k} \vec{k}'} \right|^2 \delta (\epsilon_k(0) - \epsilon_{\vec{k}'}(0)) (1 - \cos (\theta_{\vec{k} \vec{k}'}) \). (25)

Here \( \theta_{\vec{k} \vec{k}'} \) denotes the angle between \( \vec{k} \) and \( \vec{k}' \), and \( f_k' \) represents the derivative of the Fermi distribution with respect to the energy \( \epsilon_k(0) \). The set of Eq. (24) and Eq. (25) coincides with the semiclassical result provided by the Boltzmann equation [5]. In particular the factor \( 1 - \cos (\theta_{\vec{k} \vec{k}'}) \) shows that Eq. (25) represents the correct transport scattering time.

INELASTIC SCATTERING: THE FRÖHLICH POLARON

As second example we consider the Fröhlich polaron model [21, 22] where electron (\( \vec{r} \) and \( \vec{p} \) are the position and momentum operators) is scattered by phonons (\( a_q^\dagger \) the creation operator with wave number \( q \) with interaction vertex \( M_q = i \omega_0 (R_q \pi \alpha / q^2 V)^{1/2} \):

\[
H = p^2/2m + \omega_0 \sum_q a_q^\dagger a_q + \sum_q [M_q e^{i \vec{q} \cdot \vec{r}} a_q + h.c.].
\]

(26)

Here \( \alpha \) is the dimensionless coupling constant, \( R_q = (1/2m \omega_0)^{1/2} \), and \( V \) is the volume of the system.

Due to the inelastic nature of the scattering processes, the theoretical treatment is complicated [19, 23] and different approaches give different expressions even in the limit of very low temperature. These various methods usually agree in the weak coupling limit (\( \alpha \ll 1 \)) providing for the mobility (\( \mu = \sigma_{dc}/nq_e \), where \( n \) is the particle density) [2]:

\[
\mu = \frac{q_e}{2\alpha m \omega_0} N_0. \tag{27}
\]

Here \( N_0 = 1/(e^{\beta \omega_0} - 1) \) is the phonon number density.

This result can be derived from the Kubo formula [5]. The first term of the expansion of the S matrix leads to the bubble diagram including two electronic Green functions \( G(k, \omega) \), which, in turn, are obtained by Dyson’s equation at the lowest order in the electron-phonon coupling \( \alpha \). This procedure leads to \( \mu = q_e \tau / m \), where \( \tau = 1/2\alpha N_0 \omega_0 \) and then Eq. (27) is recovered. However, in this approach, \( \tau \) coincides with the electron lifetime derived from the Green function \( G(k = 0) \) and does not include the equivalent of the \( 1 - \cos (\theta_{\vec{k} \vec{k}'}) \) factor in the elastic scattering. On the other hand the Drude formula involves the transport scattering time, related to the real part of the memory function, which, in general, is not identical with the single-particle scattering time, that is related to the imaginary part of the self-energy of the electron propagator.

Another approach to derive the polaron mobility in the weak coupling limit is based on the Boltzmann equation. By neglecting the in-scattering terms contribution in the collision term, one obtains again Eq. (27) It turns out that Eq. (27) does not agree with correct solution of the Boltzmann equation in the relaxation time approximation (see discussion by Sels and Brosens [25]).

The path integrals method adds a result in disagreement with the other approaches. In the low temperature and weak coupling limits, the polaron mobility in Feynman-Hellwarth-Iddings-Platzman (FHIP) [26] approach differs from Eq. (27) by a factor of \( 3K \beta T / 2 \omega_0 \). It has been shown that the result obtained in Ref. [26] can be obtained by using the memory function formalism and the Feynman polaron model [27], so that the mobility, in this approach, suffers the problem related to the average value of \( 1/\tau \) rather than \( \tau \).

BWFOC allows trivial derivation of the correct perturbative solution of the polaron mobility. By taking into account that \( J_l = q_e p_l / m \) and \( [p_l, V] = \sum_q \delta \left( M_q e^{i \vec{q} \cdot \vec{r}} a_q - h.c. \right) \), from Eq. (28) one obtains the relaxation time \( 1/\tau_{a,k}^{(0)} = 1/\tau_{a,k}^{(0)} + 1/\tau_{e,k}^{(0)} \), where \( 1/\tau_{a,k}^{(0)} \) and \( 1/\tau_{e,k}^{(0)} \) denote the contributions coming from absorption and emission of longitudinal optical phonons respectively:

\[
1/\tau_{a,k}^{(0)} = \pi \frac{q^2}{k^2} |M_q|^2 N_0 \delta (\epsilon_k^{(0)} - \epsilon_{k+\vec{q}}^{(0)} + \omega_0) \tag{28}
\]

and

\[
1/\tau_{e,k}^{(0)} = \pi \frac{q^2}{k^2} |M_q|^2 (1 + N_0) \delta (\epsilon_k^{(0)} - \epsilon_{k-\vec{q}}^{(0)} - \omega_0). \tag{29}
\]

We emphasize that the factor \( q^2 / k^2 \), where \( q \) is the transferred momentum by phonons in the scattering, is a substitute of the factor \( 2(1 - \cos (\theta_{\vec{k} \vec{k}'}) \). Hence, BWFOC automatically introduces transport scattering time into perturbative expressions. It is remarkable that this factor, introduced phenomenologically by Fröhlich in
using the spectral representation of BWFOC. Furthermore, at low temperatures, where only momenta around $k = 0$ contribute to the mobility, one obtains $\tau_0^{(0)} \simeq r k^2 / m \omega_0$, i.e., as it is expected, the transport relaxation time $\tau_0^{(0)}$ differs by a factor $k^2 / m \omega_0$ from the single particle scattering time $\tau$. Finally, we note that in BWFOC expansion at low temperatures only the phonon absorption processes contribute to the mobility, that reflects the impossibility of the events in which a low energy polaron emits a phonon [20].

By inserting the time relaxation expression in Eq. 22 we obtain the mobility in the weak coupling regime at low temperatures as $\mu = \mu_{\text{FHIP}} 10 / 3$, i.e. the mobility differs by a numerical factor $10 / 3$ from the result of FHIP [20] and by $5 k_B T / \omega_0$ from the value obtained through the diagrammatic technique [31], i.e. Eq. 27.

In this paper we derived a new formulation of the optical conductivity which allows a trivial derivation of the Boltzmann result. The structure of BWFOC, weighting the contribution from exact eigenstates by Boltzmann occupation numbers, allows to treat weak coupling and low temperature limits trivially, which is in complete contrast with all previous formulations of the optical conductivity. Beyond recovery of the correct Boltzmann limit, BWFOC retains possibility to consider finite frequency features and perform calculations in the intermediate and strong coupling regimes. We demonstrated the power of BWFOC formulation for elastic and inelastic scattering problems.

Appendix

The new formulation of the linear response theory is based on the idea to introduce, for each of the quantum numbers $n$ labelling the eigenstates of the Hamiltonian, one relaxation or memory function $M_n(z)$:

$$
\sigma(z) = -\frac{i}{V} \sum_n p_n \frac{q_n^2 s_n}{z + iM_n(z)}. \quad (A.1)
$$

with

$$
M_n(z) = i \frac{z \Pi_n(z)}{\Pi_n(z) - q_n^2 s_n}. \quad (A.2)
$$

Here we want to prove that the quantity $\Pi_n(z) - q_n^2 s_n$ is different from zero for $\Im z \neq 0$. We observe that by using the spectral representation

$$
\Pi_n(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{3 \Pi_n(\omega)}{\omega - z}. \quad (A.3)
$$

we have, for $z = x + i\epsilon$:

$$
\Pi_n(x + i\epsilon) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{3 \Pi_n(\omega)(\omega - x + i\epsilon)}{(\omega - x)^2 + \epsilon^2}. \quad (A.4)
$$

Since $s_n$ is real, first of all we find the values $x + i\epsilon$, with $\epsilon \neq 0$, for which $\Pi_n(z)$ is real. For these values we have:

$$
\int_{-\infty}^{\infty} d\omega \frac{3 \Pi_n(\omega)}{(\omega - x)^2 + \epsilon^2} = 0. \quad (A.5)
$$

Next step is to write the denominator $D_n(z)$ of $M_n(z)$ in the complex upper half-plane for $z$ values where Eq. (A.5) is satisfied:

$$
D_n(x + i\epsilon) = -\int_{-\infty}^{\infty} d\omega \frac{3 \Pi_n(\omega)}{\pi \omega} \frac{x^2 + \epsilon^2}{(\omega - x)^2 + \epsilon^2} - q_n^2 \nu_n > 0,
$$

having taken into account that $s_n = \gamma_n + \nu_n$, $\gamma_n = \Pi_n(z = 0) / q_n^2$, $-3 \Pi_n(\omega) / \omega \geq 0$ and $\nu_n \leq 0$. This proves that $M_n(z)$ is analytic in the complex upper half-plane. A similar proof has been given [32] to justify the introduction of the memory function in the Eq. 8 of the main text.

[1] The Boltzmann Equation, Proc. Intern. Symp. 100 years Boltzmann Equation, ed. E. G. D. Cohen, and W. Thirring (Wien, Springer Verlag, 1973).
[2] N. R. Mott and H. Jones, The Theory of the Properties of Metals and Alloys, (Dover, New York, 1958).
[3] R. Kubo, J. Phys. Soc. Japan 12, 570 (1957).
[4] H. Moro, Prog. Theor. Phys. 33, 423 (1965); 34, 399 (1965).
[5] G. D. Mahan, Many Particle Physics (Plenum, N.Y., 1981).
[6] L. Van Hove, Physica (Utrecht) 21, 517 (1955).
[7] E. Verboven, Physica 26, 1091 (1960).
[8] G. V. Chester and A. Thellung, Proc. Phys. Soc. (London) 73, 765 (1959).
[9] R. Zwanzig, Phys. Rev. 124, 983 (1961).
[10] W. Götzte and P. Wölle, Phys. Rev. B 6, 1226 (1972).
[11] V. M. Kenkre and M. Dresden, Phys. Rev. A 6, 769 (1972).
[12] P. N. Argyres and J. L. Sigel, Phys. Rev. Lett. 31, 1397 (1973).
[13] S. Mukerjee and B. S. Shastry, Phys. Rev. B 77, 245131 (2008).
[14] P. F. Maldague, Phys. Rev. B 16, 2437 (1977).
[15] In particular it has been conjectured [16] that: i) integrable systems exhibit ballistical behaviour, i.e. dissipationless finite temperature conductivity, if the Drude coefficient is different from zero at $T = 0$, and remain ideal insulators, i.e. $D(T > 0) = 0$, at all temperatures if $D(T = 0) = 0$; ii) a generic nonintegrable system displays finite conductivity at finite temperature, i.e it is characterized by diffusive motion, being $D(T > 0) = 0$. We will restrict our attention to normal conductors, i.e. $\lim_{\epsilon \to 0^+} \left( \Pi(\epsilon) - q_n^2 T \right) = D(T > 0) = 0$. On the other hand we emphasize that in these systems $D(T > 0) = 0$ only if the exact eigenstates are used in the Eq. 5 so that we will retain this contribution up to the end of the calculation.
[16] H. Castella, X. Zotos, and P. Prelovsek, Phys. Rev. Lett. 74, 972 (1995); X. Zotos and P. Prelovsek, Phys. Rev. B 53, 983 (1996).
This function allows to relate the dc conductivity to physically meaningful quantities as, for example, the Einstein diffusion coefficient.\[3\]

F. M. Peeters and J. T. Devreese, Solid State Physics 38, 81 (1984).

K. M. Van Vliet, J. Math. Phys. 20, 2573 (1979).

H. Fröhlich, Phys. Rev. 79, 845 (1950).

G. De Filippis, V. Cataudella, A. S. Mishchenko, C. A. Perroni, and J. T. Devreese, Phys. Rev. Lett. 96, 136405 (2006); Eur. Phys. J. B 12, 17 (1999).

D. C. Langreth and L. P. Kadanoff, Phys. Rev. 133, A1070 (1964); G. D. Mahan, Phys. Rev. 142, 366 (1966); Y. Osaka, J. Phys. Soc. Japan 35, 381 (1973); K. K. Thornber and R. P. Feynman, Phys. Rev. B 1, 4099 (1970).

L. P. Kadanoff, Phys. Rev. 130, 1364 (1963).

D. Sels and F. Brosens, Phys. Rev. E 89, 012124 (2014).

R. P. Feynman, R. W. Hellwarth, C. K. Iddings, and P. M. Platzman, Phys. Rev. 127, 1004 (1962).

F. M. Peeters and J. T. Devreese, Phys. Rev. B 28, 6051 (1983).

H. Fröhlich, Proc. R. Soc. Lond. A 160, 230 (1937).

H. Fröhlich and N. F. Mott, Proc. R. Soc. Lond. A 171, 496 (1939). We note that, within this reference, the equations determining the transport scattering time coincide with Eq. 28 and Eq. 29 except for the factor $q^2/k^2$ that is replaced with $-2q_x/k_x$. Fröhlich and Mott themselves demonstrated, by using the energy conservation, that the factor $-2q_x/k_x$ is equivalent to the quantity $(q^2 \pm q_0^2)/k^2$ (+ (-) for one phonon emission (absorption)), where $q_0^2/2m = \omega_0$. On the other hand, the inspection of the Boltzmann equation reveals that the contribution $-2q_x/k_x$ is correct only in the elastic scattering problems (where $q_x = 0$ and, in this case, all the approaches provide the same result). We also note that the term $q_0^2/k^2$ has been neglected by Frohlich himself in ref. 28. Actually it is not clear which is the appropriate factor in the inelastic scattering problems, and, in general, it is discarded (in this way transport scattering time and electron lifetime coincide). Then the problem is open, and, so far, not solved yet. This does not allow to establish which is the correct perturbative limit for the mobility. Within BWFOC the appropriate factor both in elastic and inelastic scattering problems turns out to be $q^2/k^2$. We note, in particular, that the validity of our approach is not related to the nature of the scattering events.

Note the strange fact that in the FHIP treatment mobility is dominated by phonon emission processes.\[19\]

We emphasize that, within the SKR, the second vertex correction provides a further factor in Eq. 27 of the order of $k_B T/\omega_0$, in agreement, apart from a numerical factor, with the prediction of WBFOC (we note that WBFOC obtains this result at the lowest order).

W. Götze and P. Wolflé, J. Low Temp. Phys. 5, 575 (1971).