Alternative representation of the Kubo formula for the optical conductivity: A shortcut to transport properties

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The Kubo formula for the electrical conductivity is expressed in terms of a weighted sum of Drude-like contributions associated to the exact eigenstates of the interacting system, each characterized by its own frequency-dependent relaxation time. This alternative formulation considerably simplifies the access to the static properties (dc conductivity) and resolves the long-standing difficulty to connect the Boltzmann transport theory and the Kubo formula. In particular, at the lowest order of the perturbation theory, the correct transport scattering lifetime depending on the momentum k, which appears in the Boltzmann theory, instead of the single-electron lifetime appearing in the Green function, can be recovered. This alternative formulation is applied to (i) the elastic scattering in metals, and (ii) the inelastic scattering in the Fröhlich polaron model to obtain the exact result of the mobility in the low-temperature weak-coupling limit.

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I. INTRODUCTION

The electrical resistivity of materials is the most fundamental physical quantity. Its microscopic origin is the elastic scattering by the disorder and the inelastic scatterings by phonons or electron-electron interactions. This important topic in condensed-matter physics has been addressed by using a large number of theoretical methods [1–4]. In particular, one of the most powerful tools for investigating the transport properties is represented by the Boltzmann equation [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 [5]. Indeed, by indicating with λ a dimensionless parameter characterizing the strength of the coupling with phonon or impurities [6], even in the weak-coupling limit, contrary to many physical properties, the analysis of the dc conductivity, σ_{dc}, is not a trivial problem since σ_{dc} displays a singularity at $\lambda = 0$, i.e., $\sigma_{dc} \to \infty$ when $\lambda \to 0$ [7]. In particular, σ_{dc} can be expanded in a Laurent series in λ, near $\lambda = 0$, with the lowest-order term of the order of λ^{-2}. Although very good for the description of the transport properties at small values of λ, the Boltzmann approach cannot 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 [3], 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 the literature. One is the van Hove's $\lambda^2 t$ limit [8–10], where if the limits $\lambda \to 0$ and $t \to \infty$ (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 [4] and Zwanzig [11] and the memory function formalism [12–14]. In the following, we will call it standard formulation of the optical conductivity (SFOC). In this approach, to circumvent the divergence of σ_{dc}, the idea is to expand $1/\sigma_{dc}$ in successive powers of λ. Evaluation of the memory function at the lowest order of λ gives the classical Drude formula $\sigma_{dc} = ne^2\tau/m$, which, however, contains a relaxation time that is different from that entering into the Boltzmann solution [14]. 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 an infinite series of contributions [14].

In this paper, we derive a Boltzmann weighted formulation of the optical conductivity (BWFOC), which is equivalent to the Kubo formula [3] but has significant advantages over both the 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 an infinite series of contributions. On the other hand, BWFOC retains all advantages of SFOC, such as the possibility to consider finite frequencies and to make a systematic improvement of the result in higher orders of the interaction. We demonstrate the advantage of this alternative formulation in two problems: (i) the elastic scattering in metals, where the momentum-dependent transport scattering lifetime naturally appears in σ_{dc} without solving the Boltzmann equation, and (ii) the Fröhlich polaron problem, where the inelastic scattering by optical phonon is treated rigorously in the low-temperature weak-coupling limit in order to obtain the correct expression for the mobility.

II. KUBO FORMULA

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

$$\sigma(z) = \frac{i}{zV}\left[\Pi(z) - q_e^2\Gamma\right], \tag{1}$$

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, and the quantity Γ, in the absence of superconductivity and in the thermodynamic limit, is given by

$$q_e^2\Gamma=-\int_0^\beta d\tau\,\langle J(\tau)J(0)\rangle\,, \tag{2}$$

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

$$\Pi(z)=-i\int_0^\infty dt e^{izt}\,\langle[J(t),J(0)]\rangle\,. \tag{3}$$

In Eq. (3) [Eq. (2)], $J(t)$ [$J(\tau)$] is the (imaginary-time) Heisenberg representation of the current operator along the x axis, [,] denotes the commutator, and $\langle\,\rangle$ 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 $\epsilon\to0^+$, can be written as

$$\mathrm{Re}\sigma(\omega)=D\delta(\omega)+\sigma_{\mathrm{reg}}(\omega), \tag{4}$$

where the regular part $\sigma_{\mathrm{reg}}(\omega)$ is defined by

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

Above $p_n=e^{-\beta\epsilon_n}/Z$ is the Boltzmann weight of the eigenstate $|\psi_n\rangle$, ϵ_n is the corresponding energy, Z is the partition function, $\omega_{nm}=\epsilon_m-\epsilon_n$, $\beta=1/K_BT$, with K_B being the Boltzmann constant, and the Drude weight D, i.e., the coefficient of the zero-frequency δ function contribution, is given by [16]

$$D=\frac{\pi\beta}{V}\sum_{\substack{n\\ \epsilon_n=\epsilon_m}}\sum_m p_n\,|\langle\psi_n|\,J\,|\psi_m\rangle|^2\,. \tag{5}$$

$\sigma(\omega)$ satisfies the sum rule [18],

$$\int_{-\infty}^{\infty}d\omega\mathrm{Re}\sigma(\omega)=-\frac{\pi q_e^2\Gamma}{V}. \tag{6}$$

The SKF is the most frequently used formulation for the calculation of the quantum optical conductivity. However, we note that in this formulation, $\mathrm{Re}\sigma(\omega)$ shows a singularity at $\omega=0$ if one proceeds perturbatively. Indeed, at $\lambda=0$, $\sigma_{\mathrm{reg}}(\omega)=0$ so that only the coefficient D turns to be nonzero. As a 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.

III. MEMORY FUNCTION FORMULATION

To overcome the difficulties related to the diagrammatic techniques that have to deal with summing divergent series, the SFOC was suggested, where one represents $\sigma(z)$ in terms of a memory function $M(z)$ [12–14]:

$$\sigma(z)=-\frac{i}{V}\frac{q_e^2\Gamma}{z+iM(z)}, \tag{7}$$

with

$$M(z)=i\frac{z\Pi(z)}{\Pi(z)-q_e^2\Gamma}. \tag{8}$$

This approach, introduced earlier by Kadanoff and Martin [19], allows one to easily extract 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 [12]. Indeed, by taking into account that $\Pi(z)$ decreases as $1/z^2$ when $z\to\infty$, the first step is to expand $M(z)$ at high frequencies (short-time expansion) so that $M(z)\simeq-iz\Pi(z)/q_e^2\Gamma$. 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 $F(z)$, which is a Green function, involving the commutator between the current operator and the Hamiltonian:

$$z\Pi(z)=\frac{F(z)-F(z=0)}{z}, \tag{9}$$

with

$$F(z)=i\int_0^\infty dt e^{izt}\,\langle[J(t),H],[J(0),H]\rangle\,. \tag{10}$$

The 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 the absence of the interaction $\langle\tau\rangle_{av}$. On the other hand, in SFOC, it is $\left(\langle1/\tau\rangle_{av}\right)^{-1}$, i.e., since the SFOC approach, at the lowest order, averages the inverse relaxation times, recovery of the Boltzmann formula requires a procedure equivalent to the λ^2t limit.

IV. ALTERNATIVE 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 $z\to\infty$. Consequently, $\Pi(z)$ can be represented as a spectral integral,

$$\Pi(z)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\frac{\mathrm{Im}\Pi(\omega)}{\omega-z}. \tag{11}$$

On the other hand, $\mathrm{Im}\Pi(\omega)$ can be expressed in terms of $\Psi(z)$, the Fourier transform of symmetrized correlation function $\langle(J(t)J(0)+J(0)J(t))\rangle$:

$$\Psi(z)=-i\int_0^\infty dt e^{izt}\,\langle(J(t)J(0)+J(0)J(t))\rangle\,, \tag{12}$$

i.e., $\mathrm{Im}\Pi(\omega)=\tanh(\beta\omega/2)\mathrm{Im}\Psi(\omega)$ [20]. Successively, by introducing the Lehmann representation of the correlation function $\mathrm{Im}\Psi(\omega)$, using Eq. (11), and writing the quantity Γ 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

$$\gamma_n = -\sum_{\substack{m \\ \epsilon_n \neq \epsilon_m}} \frac{2\,|\langle\psi_n|\,J\,|\psi_m\rangle|^2}{q_e^2\omega_{nm}} \tanh\left(\frac{\beta\omega_{nm}}{2}\right), \tag{13}$$

$$\nu_n = -\frac{\beta}{q_e^2} \sum_{\substack{m \\ \epsilon_n = \epsilon_m}} |\langle\psi_n|\,J\,|\psi_m\rangle|^2\,, \tag{14}$$

and

$$\Pi_n(z) = \sum_{\substack{m \\ \epsilon_n \neq \epsilon_m}} |\langle\psi_n|\,J\,|\psi_m\rangle|^2 \tanh\left(\frac{\beta\omega_{nm}}{2}\right) f_{nm}^{(a)}(z). \tag{15}$$

Here, $f_{nm}^{(a)}(z) = \frac{1}{z-\omega_{nm}} - \frac{1}{z+\omega_{nm}}$. In terms of the microcanonical quantities $s_n = \gamma_n + \nu_n$ and $\Pi_n(z)$, the BWFOC reads

$$\sigma(z) = \sum_n p_n \sigma_n(z), \tag{16}$$

where

$$\sigma_n(z) = \frac{i}{zV}\left[\Pi_n(z) - q_e^2 s_n\right]. \tag{17}$$

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

$$\sigma_n(z) = -\frac{i}{V}\frac{q_e^2 s_n}{z + i M_n(z)}, \tag{18}$$

with

$$M_n(z) = i\frac{z\Pi_n(z)}{\Pi_n(z) - q_e^2 s_n}. \tag{19}$$

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

$$f_n(z) = \sum_{\substack{m \\ \epsilon_n \neq \epsilon_m}} \frac{|\langle\psi_n|\,[J,H]\,|\psi_m\rangle|^2}{\omega_{nm}} \tanh\left(\frac{\beta\omega_{nm}}{2}\right) f_{nm}^{(s)}(z), \tag{20}$$

which is the analogy of the introduction of the force-force correlation function in the alternative 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 also allows a nontrivial generalization to all frequencies and couplings. Namely, in all Boltzmann-like treatments, a similar formula can be derived but with frequency-independent memory function $M_n(z) = 1/\tau_n$ [21,22]. Furthermore, the quantities s_n, τ_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 alternative formulation explicitly relies on the use of eigenstates as the basis. This more limited choice allows one to explicitly incorporate 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. Equation (18) assumes the following form:

$$\sigma_n(z) = -\frac{i}{dV}\frac{q_e^2 \bar{s}_n}{z + i\bar{M}_n(z)}, \tag{21}$$

where $\bar{s}_n = \sum_{l=1}^d s_{n,l}$, $\bar{\Pi}_n(z) = \sum_{l=1}^d \Pi_{n,l}(z)$, and $\bar{M}_n(z) = iz\bar{\Pi}_n(z)/[\bar{\Pi}_n(z) - q_e^2\bar{s}_n]$. By approximating the exact eigenstates and eigenvalues with the 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 $z = i\epsilon$ and performing the limit $\epsilon \to 0^+$, one obtains

$$\sigma_{dc}^{(0)} = \frac{\beta}{dV}\sum_n p_n^{(0)}\tau_n^{(0)} \sum_{\epsilon_n^{(0)}=\epsilon_m^{(0)}} \sum_{l=1}^d \left|\langle\psi_n^{(0)}|J_l|\psi_m^{(0)}\rangle\right|^2, \tag{22}$$

where the relaxation time associated to the eigenstate of H_0 with eigenvalue ϵ_n^0 is

$$\frac{1}{\tau_n^{(0)}} = \pi\frac{\sum_{m,l}\left|\langle\psi_n^{(0)}|[J_l,V]|\psi_m^{(0)}\rangle\right|^2 \delta\left(\epsilon_n^{(0)} - \epsilon_m^{(0)}\right)}{\sum_{\epsilon_n^{(0)}=\epsilon_m^{(0)}}\sum_{l=1}^d \left|\langle\psi_n^{(0)}|J_l|\psi_m^{(0)}\rangle\right|^2}, \tag{23}$$

with J_l being the component of the current operator along the l direction. In the following, we show that on the basis of this alternative formula, some known results can be easily reproduced, but also that alternative results can be deduced in inelastic-scattering problems.

V. SCATTERING BY IMPURITIES IN METALS

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

$$\sigma_{dc}^{(0)} = -\frac{q_e^2}{dVm^2}\sum_{\vec{k}} f_k' k^2 \tau_k^{(0)}, \tag{24}$$

with

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

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 lowest-order variational solution of the Boltzmann equation [7]. In particular, the factor $1 - \cos(\theta_{\vec{k},\vec{k}'})$ shows that Eq. (25) represents the correct transport scattering time.

VI. INELASTIC SCATTERING: THE FRÖHLICH POLARON

As a second example, we consider the Fröhlich polaron model [23,24] where the electron ($\vec{r}$ and $\vec{p}$ are the position and momentum operators) is scattered by phonons ($a_{\vec{q}}^{\dagger}$ is the creation operator with wave number $\vec{q}$) with interaction vertex $M_q = i\omega_0 \left(R_p 4\pi\alpha/q^2 V\right)^{1/2}$:

$$H = p^2/2m + \omega_0 \sum_{\vec{q}} a_{\vec{q}}^{\dagger} a_{\vec{q}} + \sum_{\vec{q}} [M_q e^{i\vec{q}\cdot\vec{r}} a_{\vec{q}} + \text{H.c.}]. \quad (26)$$

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

Due to the inelastic nature of the scattering processes, the theoretical treatment is complicated [21,25] 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) [7]:

$$\mu = \frac{q_e}{2\alpha m\omega_0} N_0. \quad (27)$$

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

This result can be derived from the Kubo formula [7]. 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 α. 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, τ 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 to 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 term's contribution in the collision term [26], one again obtains Eq. (27). It turns out that Eq. (27) does not agree with the correct solution of the Boltzmann equation in the relaxation-time approximation (see discussion by Sels and Brosens [27]).

The path-integral method adds a result in disagreement with the other approaches. In the low-temperature and weak-coupling limits, the polaron mobility in the Feynman-Hellwarth-Iddings-Platzman (FHIP) [28] approach differs from Eq. (27) by a factor of $3K_BT/2\omega_0$. It has been shown that the result obtained in Ref. [28] can be obtained by using the memory function formalism and the Feynman polaron model [29], so that the mobility, in this approach, suffers the problem related to the average value of $1/\tau$ rather than τ.

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 $[p_l,V] = \sum_{\vec{q}} q_l [M_q e^{i\vec{q}\cdot\vec{r}} a_{\vec{q}} - \text{H.c.}]$, from Eq. (23) one obtains the relaxation time $1/\tau_k^{(0)} = 1/\tau_{a,k}^{(0)} + 1/\tau_{e,k}^{(0)}$, 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:

$$1/\tau_{a,k}^{(0)} = \pi \sum_{\vec{q}} \frac{q^2}{k^2} |M_q|^2 N_0 \delta\left(\epsilon_{\vec{k}}^{(0)} - \epsilon_{\vec{k}+\vec{q}}^{(0)} + \omega_0\right) \quad (28)$$

and

$$1/\tau_{e,k}^{(0)} = \pi \sum_{\vec{q}} \frac{q^2}{k^2} |M_q|^2 (1+N_0) \delta\left(\epsilon_{\vec{k}}^{(0)} - \epsilon_{\vec{k}-\vec{q}}^{(0)} - \omega_0\right). \quad (29)$$

We emphasize that the factor q^2/k^2, where $\vec{q}$ 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 1937 [30,31], had been discarded in all successive treatments but has been put back by perturbative expansion of BWFOC. Furthermore, at low temperatures, where only momenta around $k=0$ contribute to the mobility, one obtains $\tau_k^{(0)} \simeq \tau k^2/m\omega_0$, i.e., as expected, the transport relaxation time $\tau_k^{(0)}$ differs by a factor $k^2/m\omega_0$ from the single-particle scattering time τ. Finally, we note that in the BWFOC expansion at low temperatures, only the phonon absorption processes contribute to the mobility, which reflects the impossibility of the events in which a low-energy polaron emits a phonon [32].

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 [28] and by $5k_BT/\omega_0$ from the value obtained through the diagrammatic technique [33], i.e., Eq. (27).

VII. CONCLUSIONS

In this paper, we derived an alternative formulation of the optical conductivity which allows a trivial derivation of the Boltzmann result. The structure of BWFOC (16), weighting the contribution from exact eigenstates by Boltzmann occupation numbers, allows one 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 the possibility to consider finite frequency features and perform calculations in the intermediate- and strong-coupling regimes. We demonstrated the power of the BWFOC formulation for elastic- and inelastic-scattering problems.

APPENDIX

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

$$\sigma(z) = -\frac{i}{V} \sum_n p_n \frac{q_e^2 s_n}{z + iM_n(z)}, \quad (A1)$$

with

$$M_n(z) = i\frac{z\Pi_n(z)}{\Pi_n(z) - q_e^2 s_n}. \quad (A2)$$

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

$$\Pi_n(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}\Pi_n(\omega)}{\omega - z}, \tag{A3}$$

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

$$\Pi_n(x + i\epsilon) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}\Pi_n(\omega)(\omega - x + i\epsilon)}{(\omega - x)^2 + \epsilon^2}. \tag{A4}$$

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

$$\int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}\Pi_n(\omega)}{(\omega - x)^2 + \epsilon^2} = 0. \tag{A5}$$

The 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. (A5) is satisfied:

$$D_n[x(\epsilon) + i\epsilon] = -\int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}\Pi_n(\omega)}{\pi\omega}\frac{x^2 + \epsilon^2}{(\omega - x)^2 + \epsilon^2} - q_e^2 \nu_n > 0,$$

having taken into account that $s_n = \gamma_n + \nu_n$, $\gamma_n = \Pi_n(z = 0)/q_e^2$, $-\mathrm{Im}\Pi_n(\omega)/\omega \geqslant 0$, and $\nu_n \leqslant 0$. This proves that $M_n(z)$ is analytic in the complex upper half plane. A similar proof has been given [34] to justify the introduction of the memory function in Eq. (8) of the main text.

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[32] Note the strange fact that in the FHIP [28] treatment, mobility is dominated by phonon emission processes [21].

[33] We emphasize that within the SKF, the second vertex correction provides a further factor in Eq. (27) of the order of $k_B T/\omega_0$ [7], in agreement, apart from a numerical factor, with the prediction of WBFOC (we note that WBFOC obtains this result at the lowest order).

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