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THE DC ELECTRICAL CONDUCTIVITY CALCULATION PURELY FROM THE DISSIPATIVE COMPONENT OF THE AC CONDUCTIVITY I. GENERAL FORMULA DERIVATION

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The crucial item on which the whole advance in the present work rests is the recognition that the dc conductivity σ of real metals (those with scatterers) can be defined as the limit $\sigma = lim_{\omega\to 0}\sigma_R(\omega)$, where $\sigma_R(\omega)$ is the real (dissipative) component of the complex conductivity $\sigma(\omega)$, $\sigma(\omega) = \sigma_R(\omega) + i \cdot \sigma_i(\omega)$, by expelling $\sigma_i(\omega)$, the imaginary (non-dissipative) component of the linear response formula for electrical conductivity (Kubo formula) at the very start. It has been achieved by applying a specific rule of performing the limits $(\omega \to 0, s \to +0)$, where ω and s are the real and imaginary part of the complex frequency z, $z = \omega - i \cdot s$. The specific rule by which the limits $(\omega \to 0, s \to +0)$ should be performed in order to keep up the dissipative and the non-dissipative character of $\sigma_R(\omega)$ and $\sigma_i(\omega)$ respectively in the procedure of σ calculation, has been proved here in the form of a necessary and sufficient condition. This condition prescribes to take the limit $s \to +0$ before $\omega \to 0$ in order to expel from σ the non-dissipative components thoroughly, and that way it solves this heavy task. The non-dissipative component $\sigma_i(\omega)$, though not contributing directly to σ, it has an important impact to σ calculation via the equation $\lim_{\omega\to 0}\sigma_i(\omega) = 0$, determining the most relevant parameters of the carrier system such as the density of states and the internal forces are, shared by both $\sigma_i(\omega)$ and $\sigma_R(\omega)$. The power series expansion in terms of the scattering constant g for σ and the prerequisites for correct application of it are formulated.

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1 Introduction

When calculated dc electrical transport coefficients in the condensed matter are in question, the results obtained by the Boltzmann-Bloch kinetic equation approach in the relaxation time approximation (Drude formula) are not exceeded by the results obtained by the linear response theory approach, either in exactness or in simplicity of calculation. This statement has been claimed and widely expounded in many publications [1-5]. The better theoretical ground of the linear response theory approach at the start is often stated and recognized, but in practical application its advantages disappear. Why and how this happens, are the questions investigated in many publications [6-13], to mention just a few out of many others, including a few of our papers [14-20]. Our assumption is that a rather serious drop in the accuracy of calculated results happens when the Kubo formula is interpreted in terms of the relaxation time τ by following the pattern of the Drude formula, and τ itself is accounted for by the Born approximation for scattering rate. We, and recently some other authors [21-24] in their own way too, are oriented towards the improvement of the Kubo formula as a calculating tool, by avoiding any use of the Born approximation for scattering rate. A similar trend can be noticed in the electron transport phenomenon description by the use of the so-called 'balance-equation approach' [25-32]. In a recent paper [33], we have contributed to a better understanding of this matter and based on it, we have also proposed a new, improved way for the practical calculation of σ by means of the linear response theory.

The crucial attribute from which we make benefit in this investigation of the *dc* electric conduction, is the purely dissipative character of the *dc* current. The dissipative current is generally recognized by its positive entropy production [34-37]. However, in the special cases, when the current causing the external electric field $E(t)$ is of harmonic time dependence, $E(t) = E_x \cdot \cos(\omega t)$, of ω frequency and of E_x intensity oriented towards some x -axis, the dissipative component $j_R(t)$ of the whole *ac* response $j(t)$, $j_R(t) = \sigma_R(\omega) \cdot E(t) = \sigma_R(\omega) E_x \cos(\omega t)$, where $\sigma_R(\omega)$ is the time independent (frequency dependent) real part of the complex electrical conductivity $\sigma(\omega)$, can be recognized by the phase coincidence of $E(t)$ and $j_R(t)$, without any further search for entropy production. On this basis, we established in our previous work [33] that the *dc* conductivity σ, being it the special case of the *ac* conductivity, the limiting case for $\omega \to 0$, should be calculated from the Kubo formula for the *ac* conductivity $\sigma(\omega)$, or from some other linear response formula for $\sigma(\omega)$, by taking the limit $s \to +0$ before the limit $\omega \to 0$, where s is the exponent of the adiabatic switching factor, conceived as the imaginary part of the complex frequency z, $z = \omega - is$. This sequence of limits is opposite to the one adopted and applied by many other authors dealing with σ calculation from $\sigma(\omega)$ [1-10, 38-41].

The non-dissipative component $j_i(t)$ of the response $j(t)$, $j_i(t) = -\sigma_i(\omega) E_x \sin(\omega t)$, in terms of phasors is given by $j_i(t) = i\sigma_i(\omega) \cdot E(t)$, where the factor $i\sigma_i(\omega)$ is the imaginary part of the complex *ac* conductivity $\sigma(\omega)$, $\sigma(\omega) = \sigma_R(\omega) + i\sigma_i(\omega)$, $j(t) = j_R(t) + j_i(t) = \sigma(\omega) \cdot E(t)$. The commonly known fact observed experimentally that the angle $\varphi(\omega)$ closed by the two phasors $E(t)$ and $j(t)$ decreases with ω decrease, and $\varphi(\omega) \to 0$ with $\omega \to 0$, meaning that the two phasors gradually come to position of lying down on each other, therefore the component $j_i(t)$ of $j(t)$, orthogonal to $E(t)$, tends to zero, $j_i(t) = i\sigma_i(\omega) \cdot E(t) \to 0$ with $\omega \to 0$, and it can hold up only if $\lim_{\omega \to 0} \sigma_i(\omega) = 0$. It appears that $\sigma_i(\omega)$ not giving contribution to σ directly, has an important impact on σ calculation through the non-trivial equation $\lim_{\omega \to 0} \sigma_i(\omega) = 0$, whose implications are discussed to details in this research.

In the present paper we give systematic establishment of our new approach to the *dc* conductivity calculation, starting from the linear response expression in the Kubo formulation giving $\sigma(\omega)$ in terms of the velocity-velocity time correlation function [37,42,43], and by applying an accurate derivation, we reduce it to formulation giving σ in terms of the force-force time correlation function as

$$\sigma = \frac{1}{2V}\left(\frac{e}{m_e}\right)^2 \lim_{\omega\to 0}\left\{\lim_{s\to+0}\int_{-\infty}^{0} dt(-t^2)e^{st}\cos(\omega t)(F_x(t);F_x)\right\}, \tag{1}$$

$$(F_x(t);F_x) = \int_0^{\beta} d\lambda \cdot Tr\left\{\rho F_x(t-i\hbar\lambda)F_x\right\}, \tag{2}$$

$$F_x(t-i\hbar\lambda) = e^{\lambda H}e^{iHt/\hbar}F_x e^{-iHt/\hbar}e^{-\lambda H}, \tag{3}$$

$$F_x = (i\hbar)^{-1}[P_x, H], \tag{4}$$

where V is the volume, e and m_e are the free electron charge and mass respectively, P_x and H are the x -component of the carrier system's momentum vector and the Hamiltonian respectively, ρ and β are the equilibrium statistical operator and the reciprocal temperature respectively.

As compared to the Kubo formula in terms of the velocity-velocity time correlation functions, having the same formulation for the *ac* and the *dc* case [37,42,43], our eq. (1) is more convenient since it has passed through a non-trivial conversion, specific to the *dc* case. The objection on account of the Kubo formula, raised by some authors [7-10], that it does not offer a real option for practical calculation of σ, since it is too much formal, with little physics included, does not hold up for eq. (1). The most characteristic feature of the *dc* current, its dissipative character, has been explicitly included into it.

A preliminary account of the results of this work has been reported in [33]. An important advance of the present paper as compared to [33] is in finding new clear prove for our choice of the sequence in limits $(\omega \to 0, s \to +0)$ and new arguments vindicating the Taylor series expansion in g for σ on top of the earlier arguments based on Bragg diffraction (scattering) of carriers.

This paper is organized as follows. Section 2.1 gives accurate and systematic formal derivation of formula for σ from the dissipative component $\sigma_R(\omega)$ of the complex conductivity $\sigma(\omega)$. Section 2.2 presents the relationships between our and the Mori's formula for σ, that way putting our results into the context of another variant of the linear response theory giving σ in terms of the internal forces acting on the carriers. In Section 2.3 the power series expansion in the scattering constant g for σ is formulated. In Section 2.4 the physical arguments justifying the Taylor series expansion in g for σ are exposed. Section 3 is devoted to discussion and conclusions. The Appendix contains the proof of the necessary and sufficient condition, which verifies our choice for the sequence in which the limits $(\omega \to, s \to +0)$ should be performed when σ is calculated from $\sigma(\omega)$.

2 Formula for σ as it is deduced from $\sigma_R(\omega)$

2.1 Formal derivation

The Kubo formula for complex conductivity $\sigma_c(\omega)$, giving the complex response $j_c(t)$, $j_c(t) = \sigma_c(\omega)\cdot E_c(t)$, to the complex external electric field $E_c(t) = E_x \cdot \exp(i\omega t)$, in the

resolvent picture reads

$$\sigma_c(\omega) = \left(\frac{e^2}{Vm_e^2}\right)\left(\frac{1}{iz+iL}P_x; P_x\right), \tag{5}$$

where z is the complex frequency, $z = \omega - is$, with s as the imaginary part which is assumed to be an infinitesimal, representing the exponent of the so called adiabatic switching factor $exp(-s|t|)$. L is the Liouvillean superoperator [16,44], for any operator A determining its time evolution (dA/dt) via the system's Hamiltonian H,

$$\frac{dA}{dt} \equiv iLA = \frac{1}{i\hbar}[A, H], \tag{6}$$

and $((iz+iL)^{-1}P_x; P_x)$ is the generalized scalar product

$$\left(\frac{1}{iz+iL}P_x; P_x\right) = \int_0^\beta d\lambda \cdot Tr\left\{\rho\frac{1}{iz+iL}e^{\lambda H}P_x e^{-\lambda H}P_x\right\}, \tag{7}$$

with $\rho = e^{-\beta H}/Tr(e^{-\beta H})$. The operator L is Hermitian in respect to the scalar product eq. (7), and $(iz+iL)^{-1}$ is the habitual resolvent operator. By applying the operator identity

$$\frac{1}{(iz+iL)} = \frac{1}{(iz)} - \frac{1}{(iz)^2}(iL) + \frac{1}{(iz)^2}(iL)^2\frac{1}{(iz+iL)}, \tag{8}$$

to eq. (5), $\sigma_c(\omega)$ becomes

$$\sigma_c(\omega) = \frac{e^2}{Vm_e^2}\left\{\frac{1}{iz}(P_x; P_x) - \frac{1}{(iz)^2}(iLP_x; P_x) + \frac{1}{(iz)^2}\left(\frac{1}{(iz+iL)}iLP_x; (-iL)P_x\right)\right\}. \tag{9}$$

(The transition from eq. (5) to eq. (9), in the time convolution picture results from double partial integration in time t.) By straightforward calculation, for the two scalar products $(P_x; P_x)$ and $(iLP_x; P_x)$ it follows that

$$(P_x; P_x) = m_e N, \tag{10}$$

$$(iLP_x; P_x) = 0, \tag{11}$$

where N is the number of carriers in the volume V.

The complex conductivity $\sigma(\omega)$, giving the response $j(t)$, $j(t) = \sigma(\omega)\cdot E(t)$, to the real electric field $E(t) = E_x \cdot \cos(\omega t) = E_x \cdot [exp(i\omega t) + exp(-i\omega t)]/2$ reads,

$$\sigma(\omega) = \sigma_R(\omega) + i\cdot\sigma_i(\omega), \tag{12}$$

where the real (dissipative) and the imaginary (non-dissipative) components $\sigma_R(\omega)$ and $\sigma_i(\omega)$ respectively, are given through $\sigma_c(\omega)$ and $\sigma_c(-\omega)$ by the relations

$$\sigma_R(\omega) = \lim_{s\to+0}(1/2)[\sigma_c(\omega) + \sigma_c(-\omega))], \tag{13}$$

$$\sigma_i(\omega) = \lim_{s\to+0}(1/2i)[\sigma_c(\omega) - \sigma_c(-\omega))]. \tag{14}$$

The term $\sigma_c(-\omega)$ is given by an expression analogical to eq. (9) and it reads,

$$\sigma_c(-\omega) = \frac{e^2}{Vm_e^2}\left\{\frac{1}{iz_1}(P_x;P_x) - \frac{1}{(iz_1)^2}(iLP_x;P_x) + \frac{1}{(iz_1)^2}\left(\frac{1}{(iz_1+iL)}iLP_x;(-iL)P_x\right)\right\}, \tag{15}$$

where $z_1 = -\omega - is$. The right hand sides of eqs. (13) and (14) are real numbers, since $\sigma_c(-\omega)$ is the complex conjugate of $\sigma_c(\omega)$, $\sigma_c(-\omega) = (\sigma_c(\omega))^*$, and the current density $j(t)$ is a purely real number too: $j(t) = \sigma(\omega)\cdot E(t) = \sigma_R(\omega)E_x\cos(\omega t) - \sigma_i(\omega)E_x\sin(\omega t)$, where the relation $(i\cdot E(t)) = E_x\cdot\cos(\omega t + \pi/2) = -E_x\sin(\omega t)$, holding up for phasors has been assumed.

In case of $\omega \neq 0$, for $\sigma_R(\omega)$ and $\sigma_i(\omega)$, from eqs. (9), (13), (14) and (15), follow:

$$\sigma_R(\omega) = \frac{e^2}{Vm_e^2}\lim_{s\to+0}\frac{1}{2}\left\{\left[\frac{\left((iz+iL)^{-1}F_x;F_x\right)}{z^2}\right] + \left[\frac{\left((iz_1+iL)^{-1}F_x;F_x\right)}{z_1^2}\right]\right\}, \tag{16}$$

$$\sigma_i(\omega) = \frac{e^2}{Vm_e^2}\left\{\frac{-m_eN}{\omega} + \lim_{s\to+0}\frac{1}{2i}\left\{\left[\frac{\left((iz+iL)^{-1}F_x;F_x\right)}{z^2}\right] - \left[\frac{\left((iz_1+iL)^{-1}F_x;F_x\right)}{z_1^2}\right]\right\}\right\}, \tag{17}$$

where F_x is defined by

$$F_x \equiv iLP_x = (i\hbar)^{-1}[P_x, H]. \tag{18}$$

The dc conductivity σ in our approach, as formulated before in [33], is defined as the limit of $\sigma_R(\omega)$ taken for $\omega \to 0$, therefore the limit $s \to +0$ is assumed to be taken before the limit $\omega \to 0$. To obtain σ in our approach, the L'Hospital rule in z and z_1 has to be applied twice in succession to eq. (16), leading to the result

$$\sigma = \frac{-e^2}{Vm_e^2}\lim_{\omega\to0}\lim_{s\to+0}\frac{1}{2}\left\{\left(\frac{1}{(iz+iL)^3}F_x;F_x\right) + \left(\frac{1}{(iz_1+iL)^3}F_x;F_x\right)\right\}. \tag{19}$$

Here is much worthy of pointing out that eq. (19) can be derived also by taking the limits ($\omega \to 0$, $s \to +0$), not in succession like it has been done here, but simultaneously, like it has been shown in the Appendix.

Equation (19) is an exact formula for σ.

2.2 Connection to the Generalized Langevin Equation Approach

In the generalized Langevin equation approach (Mori's approach), the ac conductivity $\sigma_c^M(\omega)$ giving response to the complex external electric field $E_c(t) = E_x\cdot\exp(i\omega t)$ reads [21-24,44],

$$\sigma_c^M(\omega) = (\frac{ne^2}{m_e})\frac{1}{iz+\varphi(z)}, \tag{20}$$

where $n = (N/V)$ and $\varphi(z)$ is the Laplace transform of $\varphi(t)$,

$$\varphi(z) = \int_0^\infty dt \cdot e^{-izt} \cdot \varphi(t), \tag{21}$$

with $\varphi(t)$ as the so called orthogonal forces time correlation function

$$\varphi(t) = (f_x(t); f_x) \cdot (P_x; P_x)^{-1} = (1/Nm_e)(f_x(t); f_x). \tag{22}$$

The distinctive trait of $f_x(t)$, as compared to $F_x(t)$, $F_x(t) = \exp(iLt)F_x$, is in the time dependence of $f_x(t)$ defined by

$$f_x(t) = e^{(1-\mathcal{P})iLt} f_x, \tag{23}$$

where $\mathcal{P}$ is the projection operator [21-24,44]. Generally $F_x \neq f_x$, but in our case $F_x = f_x$. It comes from: $F_x = iLP_x = (\mathcal{P} + \mathcal{Q})iLP_x = \mathcal{P}iLP_x + \mathcal{Q}iLP_x$, where $\mathcal{Q}$ is the projection operator orthogonal to $\mathcal{P}$, $\mathcal{P} + \mathcal{Q} = 1$, and since the projection of F_x onto P_x, as it is defined by the left hand side of eq. (11) is zero, $\mathcal{P}iLP_x = (iLP_x; P_x) = 0$, our statement $\mathcal{Q}iLP_x \equiv f_x = F_x$ follows, with F_x given by eq. (18). In accordance with our definition of the *dc* conductivity given by eqs. (13) and (37) or (49), in the Mori's approach the *dc* conductivity σ^M is given by the equation

$$\sigma^M = (\frac{ne^2}{2m_e}) \lim_{\omega\to 0} \lim_{s\to+0} \left\{ \frac{1}{iz + \varphi(z)} + \frac{1}{iz_1 + \varphi(z_1)} \right\}. \tag{24}$$

To establish the relationship of σ^M to our *dc* conductivity expression, we start with the relation linking $\varphi(z)$ to $\phi(z)$ which reads [21-24,44],

$$\varphi(z) = \frac{iz \cdot \phi(z)}{iz - \phi(z)}, \tag{25}$$

where $\phi(z)$ is the Laplace transform of the full forces time correlation function $\phi(t)$, $\phi(t) = (F_x(t); F_x) \cdot (P_x; P_x)^{-1} = (1/Nm_e)(F_x(t); F_x)$. In our notation from the section before, $\phi(z)$ is given by

$$\phi(z) = (\frac{1}{Nm_e})(\frac{1}{iz + iL} F_x; F_x). \tag{26}$$

After substituting $\varphi(z)$ and $\varphi(z_1)$ by the right hand side of eq. (25) we get from eq. (24) the value of σ^M in terms of $\phi(z)$ and $\phi(z_1)$,

$$\sigma^M = (\frac{ne^2}{2m_e}) \lim_{\omega\to 0} \lim_{s\to+0} \left\{ \left[\frac{1}{iz} + \frac{1}{iz_1} \right] + \left[\frac{\phi(z)}{z^2} + \frac{\phi(z_1)}{z_1^2} \right] \right\}. \tag{27}$$

On the basis of eq. (63) proven in the Appendix, the term $[1/iz + 1/iz_1]$ in eq. (27) vanishes, and for σ^M follows

$$\sigma^M = (\frac{ne^2}{2m_e}) \lim_{\omega\to 0} \lim_{s\to+0} \left\{ \frac{\phi(z)}{z^2} + \frac{\phi(z_1)}{z_1^2} \right\}, \tag{28}$$

which, after performing the L'Hospital rule twice in succession, is identical to our eq. (19).

The virtue of eq. (24) comes up the best when started not from the Hamiltonians themselves, but from the models describing the random forces time correlation function. These forces, determining the conductivity, generally are assumed to have short living correlation and Mori himself has proposed for $\varphi(t)$ the Markoffian model, $\varphi(t) = 2\Gamma\delta(t)$, $\Gamma = 1/\tau$, where τ is the relaxation time, whose magnitude is scaled in τ_c, $\tau \sim \tau_c$, where τ_c is the correlation time, decay time of correlation, giving by eq. (21) for $\varphi(z)$,

$$\varphi(z) = \Gamma, \tag{29}$$

and by eq. (24) giving for σ^M,

$$\sigma^M = (\frac{ne^2}{m_e})\frac{1}{\Gamma} = \frac{ne^2\tau}{m_e}. \tag{30}$$

Equation (30) is nothing else but the Drude formula for dc conductivity. For this case, from eq. (25) and (29) follows

$$\phi(z) = \frac{iz\Gamma}{iz+\Gamma}, \tag{31}$$

and after substituting it into eq. (28), the result given by eq. (30) follows. Therefore, for this Markoffian model our formula eq. (**??**) gives the same result as the Mori's formula does, it gives the Drude formula.

The presumptuous resemblance of eqs. (20) and (24) to the Drude formula for the ac and the dc conductivity respectively, with $\varphi(z)$ as the reciprocal of the generalized relaxation time (memory function), has awoke an assumption that $\varphi(z)$ by its position in the denominator serves with benefit, by providing a suitable framework for getting a term of order g^{-2} for the leading term of σ, $\sigma \sim g^{-2}$, simply by Taylor series expansion in g applied to $\varphi(z)$, unlike to expressions such as eq. (28) or eq. (19) is, where $\phi(z)$ is in the numerator, not providing the mentioned benefit. The Taylor series expansion in g for $\varphi(z)$ is not at all a simple task to carry out, due to the projection operator involvement [21-24], but apart from it, from some other, more fundamental reasons, we do not prefer eq. (24) more than eq. (28) i.e. our eq. (19), in practical calculation of σ, with arguments to be exposed in the sections to follow.

2.3 Series expansion in the scattering constant

To formulate series expansion for σ, the full Hamiltonian H and the corresponding full Liouvillean L are split into two components: $H = H_0 + U$, $L = L_0 + L_u$ where L_0 and L_u belong to H_0 and U respectively, and in consent with eq. (6), for any A operator the relations: $iL_0A = (i\hbar)^{-1}[A, H_0]$, $iL_uA = (i\hbar)^{-1}[A, U]$ hold up. The partition of H we specify by taking for H_0 the part of H commuting with the momentum operator P_x, $[P_x, H_0] = 0$, and consequently $F_x^0 = iL_0P_x = 0$, while for U we take the remaining not commuting part of H, $[P_x, U] \neq 0$, and consequently $F_x^{'} = iL_uP_x \neq 0$. U is the scattering Hamiltonian, and its magnitude is proportional to some scattering constant g, and the full force F_x is reduced to the scattering force $F_x^{'}$, $F_x = F_x^0 + F_x^{'} = F_x^{'}$, with $F_x^{'}$ given by

$$F_x^{'} = (i\hbar)^{-1}\left[P_x, U\right]. \tag{32}$$

Equation (19) in terms of L_0, L_u and $F_x^{'}$, reads

$$\sigma = \frac{-e^2}{Vm_e^2} \lim_{\omega\to 0} \lim_{s\to +0} \frac{1}{2} \left\{ \left(\frac{1}{(iz + iL_0 + iL_u)^3} F_x^{'}; F_x^{'} \right) + \left(\frac{1}{(iz_1 + iL_0 + iL_u)^3} F_x^{'}; F_x^{'} \right) \right\}. \tag{33}$$

The power series in g for σ is obtained from this expression by applying power series expansion to both the resolvent

$$\frac{1}{(iz + iL_0 + iL_u)^3} = \frac{1}{(iz + iL_0)^3} \left(1 + \frac{iL_u}{iz + iL_0} \right)^{-3} = \frac{1}{(iz + iL_0)^3} \left[1 - 3\frac{iL_u}{iz + iL_0} + 6 \left(\frac{iL_u}{iz + iL_0} \right)^2 - ... \right], \tag{34}$$

and the exponential operators $e^{-\beta(H_0+U)}$ and $e^{\pm\lambda(H_0+U)}$ which are implicitly present in the generalized scalar products of eq. (33). The term of lowest order in g for σ comes from eq. (33) when both the resolvent and the mentioned exponential operators are taken in the lowest order in g:

$$\frac{1}{(iz + iL_0 + iL_u)^3} \approx \frac{1}{(iz + iL_0)^3}, \tag{35}$$

and $e^{-\beta(H_0+U)} \approx e^{-\beta H_0}$, $e^{\pm\lambda(H_0+U)} \approx e^{\pm\lambda H_0}$. Since $F_x^{'} \sim g$, the lowest order term for σ is of second order in g, $\sigma \sim g^2$, and it is given by the formula

$$\sigma = \frac{-e^2}{Vm_e^2} \lim_{\omega\to 0} \lim_{s\to +0} \frac{1}{2} \left\{ \left(\frac{1}{(iz + iL_0)^3} F_x^{'}; F_x^{'} \right)_0 + \left(\frac{1}{(iz_1 + iL_0)^3} F_x^{'}; F_x^{'} \right)_0 \right\}, \tag{36}$$

where the subscript $)_0$ means taking H_0 instead of H in the generalized scalar products.

The approximate formula for σ, eq. (36), formally emerges from the exact expression eq. (19), simply by replacing L and F_x by L_0 and $F_x^{'}$ respectively. Equation (1) is really both eqs. (19) and (36), with the resolvent picture replaced by the time convolution picture.

2.4 Physical backgrounds of the power-series in g for σ

To understand the scope of the derived formulas correctly, the argumentation as follows will help us. For the perfect crystalline metal in the single-band approximation, when $F_x = iLP_x = 0$, i.e. when the scattering forces are missing, $F_x^{'} = 0$, our eqs. (16), (17) and (19), give the results: $\sigma_R(\omega) = 0$, $\sigma_i(\omega) = (-ne^2/m_e\omega)$, and $\sigma = 0$ respectively. There is no dispute about the validity of the obtained results for $\sigma_R(\omega)$ and $\sigma_i(\omega)$; they also come out straightforward, purely by the dynamic consideration [33], since only the non-dissipative component exists in the response $j(t)$ here. However, the result for σ, $\sigma = 0$, justifying the Taylor series expansion in g for σ, needs further explanation. First we must note that the result $\sigma = 0$ is in sharp discrepancy with the Drude formula with the relaxation time τ accounted for by the Born approximation for scattering rate, proposing divergence of σ for this case, $\sigma = \infty$. Which one of these two opposite

values is to be assumed correct? We assume, the most important and most characteristic property of the *dc* current, is its purely dissipative character, meaning that the *dc* current always produces heat within the conductor itself. The only microscopic mechanism of heat production is the scattering of carriers on imperfections. Therefore, within the perfect crystalline metal without scatterers, when $g = 0$, both the heat production and the *dc* current is impossible, meaning that the *dc* conductivity σ of perfect metals is zero, $\sigma = 0$. The controversy with the *dc* conductivity of perfect metals has been extensively argued in our earlier paper [33]. The non-dissipative part of the current caused by the *dc* electric source driven on a conductor made up of a perfect metal, theoretically can be converted into an alternating (oscillating, non-dissipative) current, as a consequence of the joint action of the external *dc* electric field and the Bragg diffraction (umklapp) of carriers at the Brillouin zone boundary [45], but it is in no way a *dc* current. We assume that those theoretical expressions for σ which for conductivity of perfect metals without scatterers propose infinitely large value, give a wrong predictions in the case of perfect metals.

We assume, the correct definition of the *dc* conductivity σ is given by the expression

$$\sigma = \lim_{\omega \to 0} (\sigma_R(\omega)), \tag{37}$$

with $\sigma_i(\omega)$ omitted from the very start of σ calculation. Our present approach to σ calculation substantially is corroborated by the empirically observed fact that $\sigma_i(\omega)$ is a smooth function of ω, and for typical real metals (those with scatterers), high accuracy is characterized by

$$\sigma_i(\omega) \approx 0, \tag{38}$$

reducing the linear response relation $j(t) = \sigma(\omega) \cdot E(t)$ to

$$j(t) \approx j_R(t) = \sigma_R(\omega) \cdot E(t), \tag{39}$$

with $\sigma_R(\omega) \approx \sigma = const$, valid for all macroscopic frequencies encountered in technical use (of order up to $GHz = 10^9 Hz$), and for E_x rather weak. The smaller the frequency ω is the better the condition for the relation (38) to be fulfilled is, and finally for $\omega \to 0$ the imaginary (non-dissipative) component of $\sigma(\omega)$ disappears:

$$\lim_{\omega \to 0} \sigma_i(\omega) = 0, \tag{40}$$

valid for any real metal with scatterers where $g \neq 0$. After substituting $\sigma_i(\omega)$ by the right hand side of eq. (17), from this equation follows:

$$\lim_{\omega \to 0} \lim_{s \to +0} (\frac{-1}{2}) \left[\left(\frac{1}{(iz + iL)^2} F_x ; F_x \right) + \left(\frac{1}{(iz_1 + iL)^2} F_x ; Fx \right) \right] = N m_e, \tag{41}$$

or with the resolvent picture replaced by the time convolution picture it reads:

$$\lim_{\omega \to 0} \lim_{s \to +0} \int_{-\infty}^{0} dt \cdot (-t) \cdot \cos(\omega t) e^{st} \, (F_x(t); F_x) = N m_e, \tag{42}$$

with $(F_x(t); F_x)$ defined by eq. (2). The right hand side of eqs. (41) and (42) is a g independent positive constant $N m_e > 0$, while the left hand side is proportional to the square of the scattering constant g, therefore these equations can be obeyed only by g not too small, and consequently σ can be well defined only outside the vicinity of $g = 0$.

Instead of eq. (37), there is spread and widely used the definition of σ given by

$$\sigma = \lim_{z \to 0}(\sigma_c(z)) \tag{43}$$

with $\sigma_c(z)$ given by the right hand side of eqs. (5) or (9), where the dissipative and the non-dissipative components are not separated. This definition requires rather complex handling, which is usually called the $dc\ limit$, consisting from summation of an infinite series of terms with appreciation of the so called Van Hove's technique [1-5], whose aim is to separate and expel the non-dissipative components from the expression for $\sigma_c(z)$, which are present there if the eq. (43) is defining σ. The two limits ($\omega \to 0$, $s \to +0$) denoted by $z \to 0$ in eq. (43) are assumed to be performed with the limit $s \to +0$ taken last, after the limit $\omega \to 0$ being performed [1-10,38-41]. It is to be stressed that our approach requires the opposite sequence of these two limits. Our Appendix quite clearly indicates, that the splitting of $\sigma(z) = \sigma(\omega, s)$ into two components $\sigma(\omega, s) = \sigma_R(\omega, s) + i \cdot \sigma_i(\omega, s)$, with $\sigma_R(\omega, s)$ and $\sigma_i(\omega, s)$ defined by eqs. (47) and (48) respectively, is not enough to ensure for $\sigma_R(\omega, s)$ and $\sigma_i(\omega, s)$ to keep their dissipative and non-dissipative character respectively when $\omega \to 0$; the necessary and sufficient condition for the expression (47) for $\sigma_R(\omega, s)$ to describe exclusively the dissipative part of the current, and to contain the whole of it, is the fulfillment of the relations prescribed by eqs. (60)- (61) within the procedure of σ calculation by limits ($\omega \to 0$, $s \to +0$) simultaneously performed, which itself includes the case of the limits taking in sequence, with the rule to take $s \to +0$ before $\omega \to 0$.

The value of σ obtained from $\sigma(\omega)$ is very sensitive to the procedure by which the two limits ($\omega \to 0$, $s \to +0$) are performed. This sensitivity most obviously comes to evidence in the component here denoted by σ_D, which one meets along the σ calculation by eq. (49), and which is given by the expression:

$$\begin{aligned} \sigma_D &= \frac{e^2}{V m_e^2}(P_x; P_x)\left(\frac{1}{2}\right) \lim_{\substack{s \to +0 \\ \omega \to 0}} \left[\left(\frac{1}{iz}\right) + \left(\frac{1}{iz_1}\right)\right] \\ &= \frac{e^2 N}{2V m_e} \lim_{\substack{s \to +0 \\ \omega \to 0}} \left[\frac{1}{i\omega + s} + \frac{1}{-i\omega + s}\right]. \end{aligned} \tag{44}$$

It has been proved by eq. (63) that $\sigma_D = 0$, if eqs. (60) - (61) are appreciated. However, if these equations are not appreciated in the mentioned limits taking, then σ_D can vary within wide stretch going from zero, through finite values, up to infinity. With a convenient, but essentially an arbitrary junction of the ratio (ω/s) to the scattering constant g, one can obtain for σ_D the Drude term, like it is common in many researches of this subject [1-5]. We firmly believe that our value for σ_D, $\sigma_D = 0$, is the right one.

The eqs. (19) and (36) allow a genuine interpretation of σ, in terms of a kind of hopping conductivity. Namely, as long as a single carrier is moving solely under the influence of the dc external electric field E_x, it progresses steadily in the $k - space$ ($wavenumbers - space$), keeping the mutual position of carriers in the $k - space$ unchanged. There does not happen mixing of carriers of different k, does not happen any kind of stochastization, nigher heat production, and such carrier does not give a contribution to the dc current. Only those carriers which are scattered by the imperfections are producing stochastization and heat, and only their contribution to σ is accounted for by eqs. (19) or (36). The analogy with the hopping conduction [46,47] is obvious. The difference is, that in our case the hoppings, i.e. the scatterings, proceed in the $k - space$,

while in the ordinary, conventional hopping conduction the hoppings of carriers proceed from sites fixed in the configurational space. In our case, the steady movement of a carrier in the $k-space$ before the scattering happens, can produce significant changes in the parameters of the carrier, the parameters like the carrier's effective mass is, and other $k-dependent$ parameters, and by that way it can affect the dc conductivity significantly. Due to these circumstances, one can expect that eqs. (19) and (36), can give a good description of the dc conductivity σ from the parameters taken for the equilibrium state (for the Fermi surface), if the coupling of the external electric field is weak enough compared to the scattering forces, that way not bringing the carriers far away from the Fermi surface level before the scattering happens. In short, the conditions for the leading term of σ given by the eq. (36) to give a good approximation for σ are as follow: the coupling of the scattering Hamiltonian U is weak as compared to the H_0 Hamiltonian, and the coupling of the external electric field E_x is weak as compared to the coupling of the U Hamiltonian.

The above described interpretation of σ in terms of hoppings, helps us a lot to understand better the g dependance of σ given by eq. (36). Namely, in the ordinary (conventional) hopping conduction, σ is a rising function of the hoppings intensity, of the number of hoppings in the configurational space, i.e. σ is a rising function of some constant g characterizing the magnitude of the hopping Hamiltonian, while in our case of eq. (36) σ is a rising function of the hoppings intensity in the $k-space$ (scattering intensity), of the number of hoppings in the $k-space$, i.e. σ is a rising function of the scattering constant g characterizing the magnitude of both the Hamiltonian U and the force F_x, $U \sim g$, $F_x \sim g$. This is in obvious contradiction with the leading term of order g^{-2}, $\sigma \sim g^{-2}$, as it appearing in the framework of the Drude formula when the relaxation time τ is accounted for by the Born approximation. The problem with the expression $\sigma \sim g^{-2}$ is in the fact that this term is due to be dominant over the term of order g^2 as eq. (36) itself is, for g small, for $g = 0$ and $g \to 0$, but for $g = 0$ the expression $\sigma \sim g^{-2}$ is erroneous, and for $g \to 0$, any of the eqs.(41) or (42) is not obeyed. These facts cast shadow on the relation $\sigma \sim g^{-2}$. In the section to follow, this subject will be discussed more.

3 Discussion and Conclusions

The objective of the linear response theory to give expressions for response coefficients of many-particle systems, to the action of external dynamic fields, like external electric or magnetic fields are, has been achieved by the synthesis of both the dynamics and the statistics taking place in the system. It is generally known and recognized that those physical events which do not comprise macroscopic flows of particles or energy, like the electrical or the magnetic polarization is, are successfully described, beyond any doubts, by formulas coming from the linear response theory. The many-particle systems in these cases can be described as being in a kind of a thermodynamics equilibrium state modified by the external field, in a state with no entropy production. The Liouville equation is adequate to describe the statistics in this case. However, it is not the case with the events comprising macroscopic flow of particles or energy, like the case of an electric current is. In this case the many-particle system is in thermodynamically noneqilibrium state, with irreversible processes and entropy production taking place in the system. The Liouville equation, having the property to keep the entropy of the system invariant, presumably is inadequately applied here. The best outcome from this controversy would be the replacement

of the Liouville equation by an equation appropriate for the non-equilibrium states comprising the irreversible processes, however such an equation has not been found yet, at least there is no consensus about any of such equation [34]. To tackle this problem, a lot of efforts have been exerted so far. The best known and most appreciated are those reducing the Liouville equation to the Zwanzig's type kinetic equations by means of the projection operators [21-24,48,49].

In our present research we rely on another approach [37,50,51]. This approach is based on the replacement of the ordinary Liouville equation, one with zero on the right hand side, by the equation having an infinitesimally small, time irreversible, member on the right hand side of the Liouville equation (see eq. (2.95) in Ref. [51]). This additional member on the right hand side selects from the set of all possible statistical events only those which are irreversible ones, and implies positive entropy production. The so called adiabatic switching factor $exp(-s|t|)$, which earlier had been included into the linear response formula with formal (mathematical) arguments, to improve the convergency of the expressions, now enters into the linear response formula automatically from the very equation describing the statistics, and that way it rises the credibility of the linear response formula as it is applied to the irreversible processes. In consent with the Zubarev's review article [51], where different interpretations of the $exp(-s|t|)$ factor's effect are described, we adopt the interpretation according to which the role of the factor $exp(-s|t|)$ is to provide a mathematical framework for taking an average over the initial times t, by assuming that any moment of time t, far enough from the time instant of observation $t = 0$, is taken for the initial time, and any state of the reduced description (in our case it is any eigenstate of H_0), with the same probability is taken for the initial state; then it is followed by dynamic evolution with the H Hamiltonian for all times until the time of observation $t = 0$. This interpretation of the $exp(-s|t|)$ factor's effect is in the best conformance with the thermodynamic theory of measurement [52,53].

One of the pioneers in research of the electronic transport by means of the linear response theory H.Nakano, has emphasized [34] recently that despite the dynamic-like manners of the linear response theory, it is impossible to rely only on the dynamics arguments, when describing the electron transport in the condensed matter. This is certainly true for the dc case especially, where the time interval spent by the system to accommodate itself to the state with steady macroscopic current exists evidently. From our point of view, the eq. (40) generally is not fulfilled from the very start of the current's run in the system, since $\sigma_i(\omega)$ as it is given by eq. (17) has terms which are F_x and temperature dependent, therefore the eq. (40) is not a system's invariant, fulfilled by the same F_x at all temperatures. The first term $(-m_e N/\omega)$ within the wavy brackets of eq. (17), having origin in the non-dissipative processes, describes the largest possible non-dissipative contribution to the response component $j_i(t)$, while the two remaining terms within the brackets describe the opposite effect to the preceding one, the choking of the non-dissipative contribution due to the random forces F_x coupling. Clearly, the carrier system itself, and the parameters such as the density of states and the scattering forces F_x, determining both $\sigma_i(\omega)$ and $\sigma_R(\omega)$, must have been passed through conversion during some transition time (relaxation time) in order to satisfy the eq. (40). This conversion, governed by the eq. (40) is a thermodynamic process, not described by our formula for σ. So we can say that our formulas, eqs. (19) and (36) give σ under the condition of obeyed eq. (40).

In cases of ac electrical conduction, with very high external driving frequencies ω_{ex}, like the optical frequencies are, there is no time available for the system to carry out the above spoken conversion, vanishing of the non-dissipative current density $j_i(t)$ does not occur (the conse-

quences of the obeyed eq. (40) are not put in force), and $\sigma_R(\omega)$, the real part of $\sigma(\omega)$, describing the absorption of the electromagnetic waves can be accounted for by the Kubo formula from the parameters taken for the Fermi level. It is not the case with the low external driving frequencies, with $\omega_{ex} \to 0$. Due to these circumstances, the dc conductivity σ calculation appears to be a more difficult task than the electromagnetic waves absorption coefficient calculation.

In parallel with the current, the external electric field $E(t)$ produces electrical polarization by spatial displacement of the carrier system, whose intensity $P(t)$ is defined by

$$P(t) = \frac{1}{V} < \sum_i e x_i >, \tag{45}$$

with x_i the $i-th$ electron's position, and $< ... >$ meaning the statistical average. It is easy to show by the linear response theory that the real part of the polarization coefficient $\kappa_R(\omega)$ determining the real polarization $P_R(t)$ by the linear response expression $P_R(t) = \kappa_R(\omega) \cdot E(t)$, gives the following relation linking $\kappa_R(\omega)$ to $\sigma_i(\omega)$:

$$\kappa_R(\omega) = \sigma_i(\omega)/\omega. \tag{46}$$

¿From this equation we conclude that not obeyed eq. (40) would mean divergence of the polarization coefficient, and in the geometry of the closed electric circuit it would be unphysical. Therefore, we can say, our eqs. (19) and (36) describe the dc conductivity in the many-particle system under the boundary condition of finite polarization coefficient of the carrier system.

Full equivalence of both our and Mori's formula for σ [44] has been established in Section 2.2. There has been shown also that Drude formula for σ follows from our eq. (19) as a particular case, when the random (stochastic) forces time correlation functions are described by the Markoffian model. The models more sophisticated, like the Gaussian model is, do not lead to the Drude formula, but to some other formulas, presumably more sophisticated (see eq. (3.18) in Ref. [20]). Though it is a particular case, Markoffian model is commonly accepted as a basic in transport description generally, so is the Drude formula eq. (30). That way, σ determination is reduced to the Γ determination. But how to determine Γ? Equation (21) supplies the corresponding, but hardly the tractable scheme to do it. More tractable, most often applied way of Γ calculation is based on the Born approximation for scattering rate, by applying the Fermi's golden rule of statistical physics. From the subtle analysis as it is given by R. Peierls [54], one can see how infirm and dubious is the theoretical justification for the Born approximation in this task. We do not share this approach. Instead, we assume, an equivalent to the Fermi's golden rule, more adequate to the present task, must have been built into the linear response formula itself, and the series expansion in g as it is given by eq. (36) is a direct step of evolving it for practical use, free of both the casting of the task into a prescribed, fixed mould (Markoffian model) and of inconveniences inherent to the Born approximation. A kind of discrepancy between the Drude formula and eq. (36) exists evidently: the eq. (36) does not reproduce the pattern for σ dependence on g, $\sigma \sim g^{-2}$, as it appears from the Born approximation. Is it a shortage of eq. (36), and if it is, can it be avoided?

Alongside the eq. (36) giving the term of order g^2, the eq. (19) has the potential to give a term of order g^{-2} for the leading term of σ. In our previous works, the term of order g^{-2} for σ has been obtained by conjugating the series expansion in g applied to the correlation functions (scalar products) in eqs. (19) and (17), (see eq. (11) in Ref. [14] or eq. (1.13) in Ref. [20])).

The mentioned eq. (11) in Ref. [14] has been applied to practical calculation of σ in different systems [15,55-57], with success which compares to other conventional formulas of order g^{-2} for σ. However, by adopting eq. (11) in Ref. [14] instead of eq. (36) from this work, we have chosen the less accurate one. Namely, the eq. (11) in Ref. [14] has been obtained by taking into account only one, the lowest order term of the series in eq. (17), while by taking into account the whole series, $\alpha^{'}$ in Ref. [14] obtains the exact value which is $\alpha^{'} = iNm_e$, and after substituting it into eq. (11) in Ref. [14] it leads to eq. (36) from this work. On the ground of this experience with the series expansion in g for σ, we are tempted to state: as long as the eq. (40) is not taken into account, or it is not taken accurately, the asymptotic relation $\sigma \sim g^{-2}$ can be established, but as soon as eq. (40) is taken into account accurately, the mentioned asymptotic relation disappears and instead, the relation $\sigma \sim g^2$ steps up.

The reason for choosing the less accurate option in the preceding works was in our pattern recognition strategy aiming to obtain $\sigma \sim g^{-2}$ in consent with the Drude formula in Born approximation. Now, after the scrutiny as it is presented in our previous work [33] and afore in this work, we assume, the mentioned pattern recognition strategy is groundless. We think that it is not correct to assume that the dc transport processes always take place on the Fermi level, as this level is defined in absence of current, and to assume that the parameters describing the transport coefficient always should be taken for that level. In cases of weak scattering, small g, there are two options possible: 1) the eq. (40) cannot be obeyed and consequently, the dc current dos not exist; 2) the eq. (40) can be obeyed but only after the carrier system has passed through conversion and g, being it the state dependent quantity, raised up. We do not assume, the disobey of the relation $\sigma \sim g^{-2}$ is a shortage of eq. (36). The eq. (36) may be expected to give a correct σ from the parameters taken for the Fermi level only if the conditions specified at the end of Section 2.4 are provided. In all other cases, the conditions prescribed by eqs. (17) and (40), i.e. by any of the two equations, eq. (41) or eq. (42) should be obeyed, before σ is calculated by the linear response formula, by eqs. (19) or (36).

The need for correcting Drude formula as it appears in Born approximation became quite common in the recent decade [58]. The experimentally observed facts such as the negative temperature coefficient of resistivity and the Matthiessen's rule breakdown, having no explanation in the framework of the Drude formula and Born approximation, presumably can be well explained and tackled in terms of conductivity [59], and we assume in the framework of our eq. (36).

In spite to long and in diversity rich history of the electron transport theory, the theoretical description of transport events in bulk condensed matter, is still a challenging problem [11], and new approaches offering improvement are desirable indeed. As a matter of fact, the whole non-equilibrium thermodynamics is under the scrutiny recently. One line within this scrutiny, articulating new sound and efficient formulations from both experimental and theoretical experiences gathered so far, runs under the name of "GENERIC" [60,61]. Our present paper can be joined to this trend of research.

In summary, we point out the following conclusions. Conceptually, our approach to σ is strictly quantum mechanical. The inconsistency and discrepancy of our results with the results coming from the Boltzmann-Bloch kinetic equation in the relaxation time approximation (Drude formula), springing from different concepts and different definitions of σ, has been traced and explained here. The most remarkable and significant property of our basic eq. (19) is its purity from non-dissipative terms. ¿From the point of view of calculation efficiency, the main virtue of eq. (19), or eq. (1) equivalently, is that it allows simple Taylor series expansion in the scattering

parameter g (ordinary perturbation series expansion in the scattering Hamiltonian U), resulting in the leading term for σ given by eq. (36), unlike some other linear response formulas for σ, with the sequence of limits ($\omega \to 0, s \to +0$) opposite to ours, for which it is assumed that only series expansion in the reciprocal of g, or the Laurent series in g is allowed. The constitutive part of σ description in terms of F_x by eqs. (19) and (36) is the eq. (40) which is due to be obeyed with $\sigma_i(\omega)$ given by eq. (17). The system of two equations, eqs. (17) and (40), which is equivalent to any of the two: eq. (41) or eq. (42), presumably can serve as a genuine source, or at least as a suitable testing means, for obtaining correct values of the most relevant parameters, such as the state densities of carriers and internal forces F_x are, to be applied in σ calculation afterwards.

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Appendix

Let us introduce the definitions:

$$\sigma_R(\omega, s) = (1/2)(\sigma_c(\omega) + \sigma_c(-\omega)), \tag{47}$$

$$\sigma_i(\omega, s) = (1/2i)(\sigma_c(\omega) - \sigma_c(-\omega)), \tag{48}$$

$$\sigma_R = \lim_{\substack{s \to +0 \\ \omega \to 0}} \sigma_R(\omega, s), \tag{49}$$

$$\sigma_i = \lim_{\substack{s \to +0 \\ \omega \to 0}} \sigma_i(\omega, s), \tag{50}$$

$$j_R(t) = E_x \cdot \sigma_R(\omega, s) \cdot e^{st} \cos(\omega t), \tag{51}$$

$$j_i(t) = -E_x \cdot \sigma_i(\omega, s) \cdot e^{st} \sin(\omega t), \tag{52}$$

with $\sigma_c(\omega)$ and $\sigma_c(-\omega)$ given by eqs. (9) and (15). In eqs. (49) and (50), the two limits ($s \to +0$, $\omega \to 0$) are supposed to be performed simultaneously. In eqs. (51) and (52) $j_R(t)$ and $j_i(t)$ are the dissipative and the non-dissipative current densities respectively, but before the limits $s \to +0$ and $\omega \to 0$ have been performed. The criterion determining the rule by which the two simultaneous limits in eqs. (49) and (50) are to be performed comes from the Joule heat calculation. Namely, we are looking for such a way of performing the two simultaneous limits which gives zero value to heat P_i produced by the current density $j_i(t)$, during of a time interval T, the single period of the electric field $E(t) = E_x \cos(\omega t)$. We have,

$$\begin{aligned} P_i &= \int_{-T}^{0} j_i(t) \cdot E(t) \cdot dt = -E_x^2 \sigma_i(\omega, s) \int_{-T}^{0} e^{st} \cdot \sin(\omega t) \cos(\omega t) \cdot dt \\ &= -\frac{E_x^2 \sigma_i(\omega, s)}{2\omega} \int_{-\omega T}^{0} e^{a \cdot x} \cdot \sin(2x) \cdot dx = \frac{E_x^2 \sigma_i(\omega, s)}{\omega(a^2 + 4)} \left\{1 - e^{-2\pi a}\right\}, \end{aligned} \tag{53}$$

where $\omega T = 2\pi$, and

$$a = (s/\omega). \tag{54}$$

Now we put up the question, how do ω and s should tend to zero in the limits procedure in order to preserve the non-dissipative character of $j_i(t)$, giving $P_i = 0$. Due to $\omega \to 0$ in the denominator, the eq. (**??**) is a (0/0) expression, and it means that

$$(1 - e^{-2\pi a}) \to 0, \tag{55}$$

implying $a \to 0$. Applying series expansion to the left hand side of eq. (55),

$$(1 - e^{-2\pi a}) = 2\pi a - (1/2)(2\pi a)^2 + (1/6)(2\pi a)^3 - ..., \tag{56}$$

we get for P_i the expression

$$P_i = (\frac{E_x^2 \cdot \sigma_i(\omega, s)}{4})(\frac{2\pi a}{\omega}) \left\{1 - (1/2)(2\pi a) + (1/6)(2\pi a)^2\right\}. \tag{57}$$

The right hand side of eq. (57) will be zero if

$$(\frac{2\pi a}{\omega}) \to 0, \tag{58}$$

i.e. if

$$(\frac{2\pi a}{\omega}) = 2\pi(\frac{s}{\omega^2}) \ll 1. \tag{59}$$

Equation (59) will be satisfied for $\omega \to 0$, $s \neq 0$, if and only if ω and s fulfil the relations:

$$s = \omega^k, \tag{60}$$

where the exponent k can be any number bigger than 2,

$$k > 2. \tag{61}$$

The relations (60) - (61) prescribe the required rule to be appreciated in the two simultaneous limits in eqs. (49) and (50).

For the heat P_R, produced by the current density $j_R(t)$ given by eq. (51), in the limit ($\omega \to 0$, $s \to +0$) when the relations (60) - (61) are appreciated, we have

$$P_R = \int_{-T}^{0} j_R(t) \cdot E(t) \cdot dt = E_x^2 \sigma_R(\omega, s) \cdot \int_{-T}^{0} e^{st} \cdot \cos^2(\omega t) \cdot dt$$
$$= (\frac{E_x^2 \sigma_R(\omega, s)}{a^2 + 4}) \left[(\frac{a}{\omega}) + (\frac{2}{a\omega})\right] \cdot \left[1 - e^{-2\pi a}\right] = E_x^2 \cdot \sigma_R(\omega, s) \cdot \frac{T}{2}. \tag{62}$$

After performing the two limits ($s \to +0$ and $\omega \to 0$) in eq. (49) with appreciation of the mentioned relations (60) - (61), we obtain for P_R a correct result for the quasi-stationary electric current with the period $T = (2\pi/\omega) \to \infty$, $P_R = E_X^2 \cdot \sigma_R \cdot T/2$.

Now we can conclude: if the simultaneous limits ($\omega \to 0$, $s \to +0$) in eqs. (49) and (50) are performed with appreciation of the relations (60) - (61), then and only then we obtain σ_R

and σ_i, with the dissipative and the non-dissipative character preserved respectively. If the two limits ($s \to +0$, $\omega \to 0$) would be performed with breaking the rule prescribed by eqs. (60) and (61), the dissipative part of the *dc* conductivity would be dispersed into both σ_R and σ_i, and the definition of the *dc* conductivity, as given by the eq. (49) would not be correct. The eq. (37) where σ is calculated by sequential limits, with the rule to take $s \to +0$ before $\omega \to 0$, is a special case of eq. (49) with eqs. (60) - (61) appreciated.

The relations (60) - (61) have an important impact on the *dc* conductivity $\sigma = \sigma_R$ calculation from eq. (49), by producing the cancelling of the contribution to σ_R coming from the terms $(1/iz)(P_x; P_x)$ and $(1/iz_1)(P_x; P_x)$ contained on the right hand side of eqs. (9) and (15). It comes out straightforward on the basis of the following chain of equations:

$$\lim_{\substack{s\to+0\\ \omega\to 0}} \left[\left(\frac{1}{iz}\right) + \left(\frac{1}{iz_1}\right)\right] = \lim_{\substack{s\to+0\\ \omega\to 0}} \left[\frac{1}{i\omega + s} + \frac{1}{-i\omega + s}\right]$$
$$= \lim_{\substack{s\to+0\\ \omega\to 0}} \left[\frac{2s}{\omega^2 + s^2}\right] = \lim_{\omega\to 0} \omega^{k-2} \left[\frac{2}{1 + \omega^{2k-2}}\right] = 0, \tag{63}$$

where the relations (60) - (61) have been applied.

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