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THE DC ELECTRICAL CONDUCTIVITY CALCULATION PURELY FROM THE DISSIPATIVE COMPONENT OF THE AC CONDUCTIVITY II. FORMULA FOR CONDUCTORS WITH STATIC SCATTERERS

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While the first part of this work was devoted to the conceptual and most crucial questions of the dc electrical conductivity σ, the present second part is devoted to the technical questions of the theory, to elaboration of the concept to the particular systems. The conducting system to be investigated has been defined here by five suppositions (postulates), rather general to include the systems of practical interest, like metals in solid and liquid phase are, and the amorphous conductors, like the alloys and conducting glasses are. A formula for dc conductivity calculation has been derived, which gives σ in terms of the matrix elements $|<\Psi_{k+q}|\mathbf{F}|\Psi_k>|^2$, where $\mathbf{F}$ is the scattering force, and Ψ_{k+q}, Ψ_k, are the Bloch functions. For the case when Bloch functions are approximated by plane waves, an approximate formula for σ has been obtained in a more tractable form. Specific to our concept is the inclusion of an equation constitutive to σ calculation, which also has been elaborated for the considered system, to the stage suitable for practical application. σ calculation in conjunction with the mentioned constitutive equation is the most important innovative element of our concept, and we expect it will lead to substantial advance in research of this subject.

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1 Introduction

In the first part of this paper [1], hereafter referred to as I., the dc regime of electrical current, and the theoretical determination of the corresponding transport coefficient, the dc conductivity σ, has been outlined with the special attention to those issues which still are disputable. An example of such kind is the question, what is the numerical value of the dc electrical conductivity σ of perfect systems without scatterers, like the perfect crystalline metal is. From the

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critical analysis and observations presented in a number of works [2–4], and from the experience we have got so far from the theoretical investigation of this subject by means of the linear response theory [5–8], we came to a synthesis, to a concept, with two main points as follow:

1) Instead of the usual formulation of the Kubo formula giving σ in terms of the velocity-velocity time correlation function [9], we prefer the formulation in terms of the force-force time correlation function as

$$\sigma = \frac{1}{6V}\left(\frac{e}{m_e}\right)^2 \lim_{\omega\to 0}\left\{\lim_{s\to+0}\int_{-\infty}^{0} dt(-t^2)e^{st}\cos(\omega t)(\mathbf{F}(t);\mathbf{F})\right\}, \tag{1}$$

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

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

$$\mathbf{F} = (i\hbar)^{-1}[\mathbf{P}, H], \tag{4}$$

where V is the volume, e and m_e are the free electron charge and mass respectively, $\mathbf{P}$ and H are the carrier system's momentum vector and the Hamiltonian, ρ and β are the equilibrium statistical operator and the reciprocal temperature respectively. (Isotropic conducting system is assumed here.)

2) The second point of exceptional interest here is the vanishing of the non-dissipative component $\sigma_i(\omega)$ of the full ac electrical conductivity $\sigma(\omega)$, with the frequency vanishing,

$$\lim_{\omega\to 0}\sigma_i(\omega) = 0.$$

From the linear response formula for $\sigma_i(\omega)$ we have derived a certain formula (see eq. [41] in I.), which in the time convolutions picture reads,

$$\lim_{\omega\to 0}\lim_{s\to+0}\int_{-\infty}^{0} dt\cdot(t)\cdot\cos(\omega t)e^{st}(\mathbf{F}(t);\mathbf{F}) = 3Nm_e. \tag{5}$$

This is the formula we call, the constitutive equation to σ calculation. We assume, this equation provides the information relating the specific alterations the system is submitted to while the dc current is running in it, and it cannot be left out of σ calculation. To the best of our knowledge, eq. (5) newer has been used within procedure of σ calculation so far.

This paper is organized as follows. In Section 2.1 the model of the conducting system with static scatterers is defined, and the basic terms are commented and evolved. In Section 2.2, the smoothing of singularities and the analytical integration over the wavenumbers describing the quantum states is outlined, as it is applied to the case of most general isotropic matrix elements of the scattering forces, and in section 2.3 the eq. (5) is evolved. Sections 3.1 and 3.2 convert the general result for σ into more tractable ones for the particular cases of the scattering matrix and carriers energy. Section 4 is devoted to short discussion and conclusions of results.

2 Formula for σ in case of static scatterers

2.1 Model System

We assume

1. The conduction electrons, hereafter called carriers, can be described in terms of the single-band system. The imperfections disturbing the perfect crystalline structure are static.

2. Both the carrier's wavefunction Ψ_k and energy ε_k are well defined with wavenumber k.

3. The energy ε_k obeying spherical symmetry is a monotonically increasing function of k.

4. The first derivative of the carriers' partition function n_k (the Fermi distribution function), can be substituted by the delta function

$$\left(\frac{-\partial n_k}{\partial \varepsilon_k}\right) = \delta(\varepsilon_k - \varepsilon_f). \tag{6}$$

5. Radius k_G of the k space, and the energy ε_G corresponding to k_G, exceed the Fermi radius k_f and the Fermi energy ε_f respectively, much enough to obey the relation

$$(\varepsilon_G - \varepsilon_f) \gg k_B T, \tag{7}$$

where k_B and T are Boltzmann's constant and temperature respectively.

The above five postulates provide firm ground for rigorous theoretical derivation in what follows here, and do not restrict the applicability of obtained results to a certain real systems.

In presence of imperfections, the exact eigenfunctions Ψ and eigenvalues ε of the full Hamiltonian H, cannot generally be determined solely by the wavenumber k. In the above supposition 2, we assume that Ψ_k and ε_k are eigenfunctions and eigenvalues for some H_0 Hamiltonian, the closest one to H, which allows an exact description in terms of k. A favorable choice for H_0 includes, besides the periodic potential of the perfect crystalline lattice U_p, also the periodic component $U_{im}^{'}$, $U_{im}^{'} = U_{im}^{'}(\mathbf{r})$, of the full imperfections Hamiltonian $U_{im} = U_{im}(\mathbf{r})$. $U_{im}^{'}$ is determined by the Fourier series $U_{im}^{'} = U_{im}^{'}(\mathbf{r}) = \sum_\kappa (U_{im})_\kappa \cdot \exp(i\kappa \cdot \mathbf{r})$, where the summation runs over all reciprocal lattice vectors κ, and the coefficients $(U_{im})_\kappa$ are determined from U_{im} by the Fourier integrals $(U_{im})_\kappa = (1/V)\int_V d^3\mathbf{r} \cdot U_{im}(\mathbf{r}) \cdot \exp(-i\kappa \cdot \mathbf{r})$. Therefore, the sum $(U_p + U_{im}^{'})$ obeys the translational lattice symmetry, and for H_0 we take, $H_0 = T + U_p + U_{im}^{'}$, where T is the kinetic energy operator. The eigenvalues ε_k of this H_0 are a kind of the carrier's energy renormalized due to U_{im} coupling, and the eigenfunctions Ψ_k of H_0 are Bloch's functions. This H_0 can be named the Hamiltonian of the effectively perfect crystal (periodic structure, a hypothetical perfect crystal), which includes even the liquid state when U_p is completely annulled by $U_{im}^{'}$, i.e. when $U_p + U_{im}^{'} = 0$. We transcribe the total Hamiltonian $H = T + U_p + U_{im}$, to the form

$$H = H_0 + U, \tag{8}$$

where U is the non-periodic part of U_{im}, $U = U_{im} - U_{im}^{'}$. Of utmost importance for H_0 is its property to commute with the momentum operator $\mathbf{P}$, while observed in the Hilbert space of the single-band system [10],

$$[\mathbf{P}, H_0] = 0. \tag{9}$$

The component U from the right hand side of eq. (8) generally does not commute with the momentum operator $\mathbf{P}$, $[\mathbf{P}, U] \neq 0$. Consequently, the force $\mathbf{F}$ defined by eq. (4) is reduced to

$$\mathbf{F} = -\nabla_{\mathbf{r}} \left(U(\mathbf{r}) \right). \tag{10}$$

It should be stressed that $U = U(\mathbf{r})$ in this formula is supposed to obey all the properties of a stochastic Hamiltonian [11]. The concept of transport coefficients calculation running under the name of Virtual-crystal approximation [12], applies to the full Hamiltonian H a splitting similar to our given by eq. (8).

The matrix element $< \Psi_{k+q}|\mathbf{F}|\Psi_k >$ between Bloch's functions [13], Ψ_{k+q} and Ψ_k, with $\Psi_{k+q} = V^{-1/2} \cdot u_{k+q}(\mathbf{r}) \cdot \exp(i(\mathbf{k}+\mathbf{q}) \cdot \mathbf{r})$, and $\Psi_k = V^{-1/2} \cdot u_k(\mathbf{r}) \cdot \exp(i\mathbf{k} \cdot \mathbf{r})$ reads

$$< \Psi_{k+q}|\mathbf{F}|\Psi_k >= -\frac{1}{V} \int_V d^3r \cdot u^*_{k+q}(\mathbf{r}) u_k(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \nabla_{\mathbf{r}} \left(U(\mathbf{r}) \right). \tag{11}$$

The time correlation function $(\mathbf{F}(t); \mathbf{F})$ defined by eq. (2) in terms of the second quantization reads

$$(\mathbf{F}(t), \mathbf{F}) = \sum_{k,q,k',q'} < \Psi_{k+q}|\mathbf{F}|\Psi_k >< \Psi_{k'+q'}|\mathbf{F}|\Psi_{k'} > \cdot K$$
$$\cdot \int_0^\beta d\lambda \cdot \exp(\lambda(\varepsilon_{k+q} - \varepsilon_k)) \cdot \exp(it(\varepsilon_{k+q} - \varepsilon_k)/\hbar), \tag{12}$$

where K is the thermodynamic average of field operators

$$K =< a^+_{k+q} a_k a^+_{k'+q'} a_{k'} >, \tag{13}$$

with a^+_{k+q} and $a^+_{k'+q'}$ as creation, and a_k and $a_{k'}$ as annihilation operators of carriers respectively.

Standard calculation of the right hand side of eq. (13) by Wick's theorem [14] (Bloch-DeDominicis) gives,

$$(\mathbf{F}(t); \mathbf{F}) = \sum_{k,q} |< \Psi_{k+q}|\mathbf{F}|\Psi_k >|^2 \left(\frac{n_k - n_{k+q}}{u} \right) \left(e^{(iut/\hbar)} + e^{-(iut/\hbar)} \right). \tag{14}$$

where $n_k =< a^+_k a_k >$ and $n_{k+q} =< a^+_{k+q} a_{k+q} >$, are the Fermi distribution functions for carriers, and u is the energy difference

$$u = \varepsilon_{k+q} - \varepsilon_k. \tag{15}$$

(Spin degeneration is included in eq. (14)). By substituting eq. (14) into eq. (1), after performing the integration in t, we obtain for σ the expression,

$$\sigma = \left(\frac{i\hbar^3 e^2}{6Vm_e^2} \right) \lim_{\omega \to 0} \left\{ \lim_{s \to +0} \sum_{k,q} |< \Psi_{k+q}|\mathbf{F}|\Psi_k >|^2 \left(\frac{n_k - n_{k+q}}{u} \right) \cdot \right.$$
$$\left. \left[\left(\frac{1}{(u + \omega\hbar + i\hbar s)^3} - \frac{1}{(u + \omega\hbar - i\hbar s)^3} \right) + \left(\frac{1}{(u - \omega\hbar + i\hbar s)^3} - \frac{1}{(u - \omega\hbar - i\hbar s)^3} \right) \right] \right\}. \tag{16}$$

In the derivation to follow the assumption is applied that $|< \Psi_{k+q}|\mathbf{F}|\Psi_k >|^2$ is a certain function $|\mathbf{F}(k,q,k_1)|^2$, depending on the three vector lengths: k, q and k_1, ($k_1 = |\mathbf{k}+\mathbf{q}|$, see Fig. 1.),

$$|\mathbf{F}(k,q,k_1)|^2 = |< \Psi_{k+q}|\mathbf{F}|\Psi_k >|^2. \tag{17}$$

This assumption applies to the most general case of scattering, cylindrically symmetric in reference to the incoming carrier's velocity as the symmetry axis.

The limit $s \to +0$ in eq. (16) is supposed to be performed by the formula [15]

$$\lim_{s\to+0}\left(\frac{1}{(u\pm\omega\hbar+i\hbar s)^3}-\frac{1}{(u\pm\omega\hbar-i\hbar s)^3}\right)=(-i\pi)\frac{\partial^2\left(\delta(u\pm\omega\hbar)\right)}{\partial u^2}. \tag{18}$$

With these assumptions, eq. (16) reads,

$$\sigma=\lim_{\omega\to0}\left(\frac{\hbar^3Ve^2}{48\pi^3m_e^2}\right)\int_0^{q_G}dq\cdot q^2\int_0^{k_G}dk\cdot k^2\int_0^{\pi}d\vartheta\sin(\vartheta)|\mathbf{F}(k,q,k_1)|^2 \cdot\left(\frac{n_k-n_{k+q}}{u}\right)\left[\frac{\partial^2\left(\delta(u+\omega\hbar)\right)}{\partial u^2}+\frac{\partial^2\left(\delta(u-\omega\hbar)\right)}{\partial u^2}\right], \tag{19}$$

where the summation in **k** and **q** have been converted into integration in **k** and **q**, of course with the thermodynamic limit assumed to be performed beforehand.

2.2 Singularity smoothing and analytical integration for σ

Having already performed the limit $s \to +0$, we are faced with the limit taking $\omega \to 0$ [1]. Some authors [16] argue for precaution when $\omega \to 0$ is to be taken under the argument of the δ-function. With full appreciation of this warning, in our case, the limit $\omega \to 0$ can be performed in eq. (19) simply by putting there $\omega = 0$. The smoothing of the singularity will be carried out here by a series of partial integrations, which brings the derivative sign over from the δ-function to the remaining non-singular part of the integrand.

The three-dimensional integration in eq. (19) will be performed sequentially, in three steps by the scheme as follows

$$\sigma = \sigma_0 \cdot L \tag{20}$$

$$\sigma_0 = \left(\frac{V\hbar^3e^2}{48\pi^3m_e^2}\right), \tag{21}$$

$$L = \int_0^{q_G} dq\cdot q\cdot J(q), \tag{22}$$

$$J(q) = \int_0^{k_G} dk\cdot k\cdot I(k,q), \tag{23}$$

$$I(k,q) = 2kq\int_0^{\pi}d\vartheta\sin(\vartheta)|\mathbf{F}(k,q,k_1)|^2\left(\frac{n_k-n_{k+q}}{u}\right)\frac{\partial^2\left(\delta(u)\right)}{\partial u^2}. \tag{24}$$

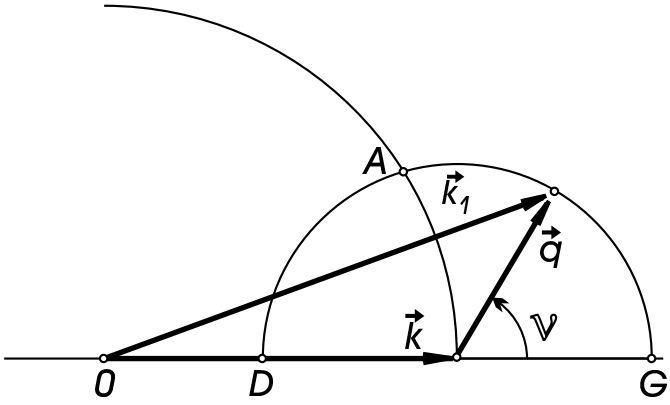

Fig. 1. The geometry of wavenumbers (vectors) $\mathbf{k}$, $\mathbf{q}$ and $\mathbf{k}_1$.

The integration in ϑ goes first in eq. (24) by keeping k and q constant, then the integration in k in eq. (23) comes by keeping q constant, and finally the integration in q proceeds in eq. (22).

Figure 1. shows the contour of integration in ϑ: it is a semicircle of radius q, with the centre at the top of vector $\mathbf{k}$.

It is convenient here to convert the integration in ϑ into an integration in u, by making use of eq. (15), from which follows

$$\sin(\vartheta) \cdot d\vartheta = \left(\frac{-k_1}{kq}\right) \left(\frac{\partial \varepsilon_{k_1}}{\partial k_1}\right)^{-1} \cdot du. \tag{25}$$

Substituting eq. (25) into eq. (24) we get

$$I(k,q) = \int_{u_D}^{u_G} du \left[D(k,q,k_1) \left(\frac{n_k - n_{k+q}}{u}\right)\right] \frac{\partial^2 \left(\delta(u)\right)}{\partial u^2}, \tag{26}$$

$$D(k,q,k_1) = 2k_1 \cdot |\mathbf{F}(k,q,k_1)|^2 \cdot \left(\frac{\partial \varepsilon_{k_1}}{\partial k_1}\right)^{-1}, \tag{27}$$

where the integration limits u_D and u_G are the energy differences defined by eq. (15), when the top of vector $\mathbf{k}_1$, is at D and G in Fig. 1. respectively.

After applying double partial integration in u, the integral in eq. (26) is rewritten as

$$I(k,q) = I_2^*(k,q) + I_1^*(k,q) + I_0^*(k,q), \tag{28}$$

where

$$I_2^*(k,q) = \left\{ \left[D(k,q,k_1) \left(\frac{n_k - n_{k+q}}{u}\right)\right] \frac{\partial \delta(u)}{\partial u} \right\} \Bigg|_{u_D}^{u_G}, \tag{29}$$

$$I_1^*(k,q) = -\left\{\frac{\partial}{\partial u}\left[D(k,q,k_1)\left(\frac{n_k - n_{k+q}}{u}\right)\right]\cdot\delta(u)\right\}\Bigg|_{u_D}^{u_G}, \tag{30}$$

$$I_0^*(k,q) = \int_{u_D}^{u_G} du \frac{\partial^2}{\partial u^2}\left[D(k,q,k_1)\left(\frac{n_k - n_{k+q}}{u}\right)\right]\cdot\delta(u). \tag{31}$$

The integration in eq. (31) is trivial due to the delta function presence in the integrand, reducing eq. (31) to

$$I_0^*(k,q) = \left\{\frac{\partial^2}{\partial u^2}\left[D(k,q,k_1)\left(\frac{n_k - n_{k+q}}{u}\right)\right]\right\}_{u=0}. \tag{32}$$

As a result of the calculation shown in *Appendix* we get

$$I_0^*(k,q) = \begin{cases} I_0(k,q) & ,q \le 2k \\ 0 & ,q > 2k \end{cases} \tag{33}$$

$$I_0(k,q) = \left[D_1(k,q,k_1)\left(\frac{-\partial n_k}{\partial\varepsilon_k}\right) + D_2(k,q,k_1)\left(\frac{-\partial^2 n_k}{\partial\varepsilon_k^2}\right) + D_3(k,q,k_1)\left(\frac{-\partial^3 n_k}{\partial\varepsilon_k^3}\right)\right], \tag{34}$$

where

$$\begin{aligned} D_1(k,q,k_1) = &\left[\left(\frac{\partial^2|\mathbf{F}(k,q,k_1)|^2}{\partial k_1^2}\right)_{k1=k} + \left(\frac{\partial|\mathbf{F}(k,q,k_1)|^2}{\partial k_1}\right)_{k1=k}\left(\frac{-b(k)}{a(k)}\right)\right]\left(\frac{3G_3(k)}{a^2(k)}\right) \\ &+ \left(\frac{\partial|\mathbf{F}(k,q,k_1)|^2}{\partial k_1}\right)_{k1=k}\left(\frac{2G_2(k)}{a(k)}\right) + \left(|\mathbf{F}(k,q,k_1)|^2\right)_{k1=k} G_1(k), \end{aligned} \tag{35}$$

$$D_2(k,q,k_1) = \left(\frac{\partial|\mathbf{F}(k,q,k_1)|^2}{\partial k_1}\right)_{k1=k}\left(\frac{3G_3(k)}{a(k)}\right) + \left(|\mathbf{F}(k,q,k_1)|^2\right)_{k1=k} G_2(k), \tag{36}$$

$$D_3(k,q,k_1) = \left(|\mathbf{F}(k,q,k_1)|^2\right)_{k1=k} G_3(k), \tag{37}$$

with

$$G_1(k) = \left(\frac{1}{a(k)}\right)^3\left[(6k)\left(\frac{b(k)}{a(k)}\right)^2 + (-6)\left(\frac{b(k)}{a(k)}\right) + (-2k)\left(\frac{c(k)}{a(k)}\right)\right], \tag{38}$$

$$G_2(k) = \left(\frac{1}{a(k)}\right)^2\left[(-2k)\left(\frac{b(k)}{a(k)}\right) + 2\right], \tag{39}$$

$$G_3(k) = \left(\frac{1}{a(k)}\right)\left(\frac{2k}{3}\right), \tag{40}$$

where

$$a(k) = \left(\frac{\partial\varepsilon_k}{\partial k}\right), \tag{41}$$

$$b(k) = \left(\frac{\partial^2 \varepsilon_k}{\partial k^2} \right), \tag{42}$$

$$c(k) = \left(\frac{\partial^3 \varepsilon_k}{\partial k^3} \right). \tag{43}$$

It is easy to notice from the Fig. 1. that the circle with the radius $q > 2k$ never cuts the semicircle with radius k, therefore the energy conservation law in the scattering event meaning $u = 0$, i.e. $k = k_1$, cannot be obeyed for $q > 2k$, therefore $I_0^*(k, q) = 0$ for $q > 2k$, like it is given in eq. (33).

The integration in k by eq. (23) is in turn now. It is convenient to split the calculation of $J(q)$ into three components as follows:

$$J(q) = J_2(q) + J_1(q) + J_0(q), \tag{44}$$

where

$$J_2(q) = \int_0^{k_G} dk \cdot k \cdot I_2^*(k, q), \tag{45}$$

$$J_1(q) = \int_0^{k_G} dk \cdot k \cdot I_1^*(k, q), \tag{46}$$

$$J_0(q) = \int_{(q/2)}^{k_G} dk \cdot k \cdot \left\{ D_1(k, q, k_1) \left(\frac{-\partial n_k}{\partial \varepsilon_k} \right) + D_2(k, q, k_1) \left(\frac{-\partial^2 n_k}{\partial \varepsilon_k^2} \right) + D_3(k, q, k_1) \left(\frac{-\partial^3 n_k}{\partial \varepsilon_k^3} \right) \right\}. \tag{47}$$

The eq. (47) has been obtained by substituting for $I_0^*(k, q)$ the right hand sides of eqs. (33) and (34).

The calculation of $J_2(q)$ has lead to the result

$$J_2(q) = 0. \tag{48}$$

It is easy to anticipate this result even without a detailed calculation, if keeping in mind that the derivative of the delta function in eq. (29), $(\partial \delta(u)/\partial u)$, is an odd function of u and strongly is peaked within a narrow (infinitesimal) interval round the point $u = 0$, while the remaining factors of the integrand in eq. (29) are smooth functions of u.

In calculating $J_1(q)$, one has to start with eq. (30). For any $q > 0$ the upper integration limit u_G is greater than zero, $u_G > 0$, and due to the multiplier $\delta(u)$, in eq. (30), there is no contribution to $I_1^*(k, q)$ coming from u_G. The lower integration limit u_D can give a non-zero contribution to $I_1^*(k, q)$ when $u_D = 0$, and from Fig. 1. one can see that it happens in the point $k = q/2$, for any $q > 0$. Therefore, to account $J_1(q)$, the right hand side of eq. (30), as it is taken for u_D, has to be inserted into eq. (46), and afterwards the integration itself has to be performed with the special care in the vicinity of the point $k = q/2$, with q as a given constant. That way

the singularity of the integrand in eq. (46) has been smoothed by the integration in k, leading to the result as follows

$$J_1(q) = \left\{ \frac{1}{a(k)^3} \left[\left(k - k^2 \frac{b(k)}{a(k)} \right) |F(k,q,k_1)|^2 + k^2 \frac{\partial}{\partial k_1} |F(k,q,k_1)|^2 \right] \cdot \left(\frac{-\partial n_k}{\partial \varepsilon_k} \right) + \frac{k^2}{2a(k)^2} |F(k,q,k_1)|^2 \left(\frac{-\partial^2 n_k}{\partial \varepsilon_k^2} \right) \right\}_{k_1 = k = q/2}. \quad (49)$$

The integrand in eq. (47) is singularity-free. By applying the relation

$$dk = \frac{d\varepsilon_k}{a(k)}, \quad (50)$$

resulting from eq. (41), $J_0(q)$ is rewritten as

$$J_0(q) = \int_{\varepsilon_{q/2}}^{\varepsilon_G} d\varepsilon_k \left(\frac{k}{a(k)} \right) \cdot \left\{ D_1(k,q,k_1) \left(\frac{-\partial n_k}{\partial \varepsilon_k} \right) + D_2(k,q,k_1) \left(\frac{-\partial^2 n_k}{\partial \varepsilon_k^2} \right) + D_3(k,q,k_1) \left(\frac{-\partial^3 n_k}{\partial \varepsilon_k^3} \right) \right\}. \quad (51)$$

where the upper integration limit ε_G is defined in supposition 5 by eq. (7), and the lower integration limit $\varepsilon_{q/2}$ is the energy ε_k, taken for $k = q/2$. By applying a series of partial integrations in ε_k, the derivatives $(-\partial^2 n_k / \partial \varepsilon_k^2)$ and $(-\partial^3 n_k / \partial \varepsilon_k^3)$, standing as multipliers in some members of the integrand in eq. (51) can be reduced to $(-\partial n_k / \partial \varepsilon_k)$, and then the integration itself is performed easily by the use of eq. (6).

The final result for $J(q)$ obtained this way is given in the sum as follows:

$$J(q) = C^*(q) + J^*(q), \quad (52)$$

where

$$C^*(q) = \begin{cases} C(q) & , q \le 2k_f \\ 0 & , q > 2k_f \end{cases} \quad (53)$$

$$C(q) = \frac{32 m_1^4}{3\hbar^8} \left\{ \frac{1}{16 k_f^4} \left[-1 - 4\left(\frac{m_1}{m_2}\right) + 5\left(\frac{m_1}{m_2}\right)^2 - 2\left(\frac{m_1}{m_3}\right) \right] \left(|\mathbf{F}(k,q,k_1)|^2 \right)_{\substack{k=k_f \\ k_1=k_f}} + \frac{1}{8 \cdot k_f^3} \left[1 - 2\left(\frac{m_1}{m_2}\right) \right] \cdot \left(\frac{\partial |\mathbf{F}(k,q,k_1)|^2}{\partial k} \right)_{\substack{k=k_f \\ k_1=k_f}} + \frac{1}{16 \cdot k_f^2} \left[2 \left(\frac{\partial^2 |\mathbf{F}(k,q,k_1)|^2}{\partial k^2} \right)_{\substack{k=k_f \\ k_1=k_f}} - \left(\frac{\partial^2 |\mathbf{F}(k,q,k_1)|^2}{\partial k \partial k_1} \right)_{\substack{k=k_f \\ k_1=k_f}} \right] \right\}, \quad (54)$$

$$m_1 = \hbar^2 k_f \left(\frac{\partial \varepsilon_k}{\partial k} \right)^{-1}_{k=k_f}, \quad (55)$$

$$m_2 = \hbar^2 \left(\frac{\partial^2 \varepsilon_k}{\partial k^2} \right)^{-1}_{k=k_f}, \tag{56}$$

$$m_3 = \hbar^2 k_f^{-1} \left(\frac{\partial^3 \varepsilon_k}{\partial k^3} \right)^{-1}_{k=k_f}. \tag{57}$$

$$J^*(q) = \left\{ \left(\frac{k^2}{3 \cdot a(k)^3} \right) \left\{ \left(\frac{\partial |\mathbf{F}(k,q,k_1)|^2}{\partial k_1} \right)_{k_1=k} - 2 \left(\frac{\partial |\mathbf{F}(k,q,k_1)|^2}{\partial k} \right)_{k_1=k} + \left(\frac{-1}{k} + \frac{b(k)}{a(k)} \right) \cdot \left(|\mathbf{F}(k,q,k_1)|^2 \right)_{k_1=k} \right\} \cdot \left(\frac{\partial n_k}{\partial \varepsilon_k} \right) \right\}_{k=q/2} + \left\{ \frac{k^2}{6 \cdot a(k)^2} \left(|\mathbf{F}(k,q,k_1)|^2 \right)_{k_1=k} \cdot \left(\frac{\partial^2 n_k}{\partial \varepsilon_k^2} \right) \right\}_{k=q/2}. \tag{58}$$

In m_1 and m_2 we recognize the velocity mass and the dynamic mass of carriers respectively, taken for Fermi level.

To obtain L, the integration in q by eq. (22) is to be performed. It is convenient to split the calculation of L into two components as follow,

$$L = L_0 + L_1, \tag{59}$$

where

$$L_0 = \int_0^{2k_f} dq \cdot q \cdot C^*(q), \tag{60}$$

$$L_1 = \int_0^{q_G} dq \cdot q \cdot J^*(q), \tag{61}$$

with $C^*(q)$ and $J^*(q)$ given by eqs. (53) and (58) respectively.

The integration for L_0 is simple and it proceeds in terms of q, while the integration for L_1 is a bit tricky and it proceeds with the integration variable q substituted by ε_k,

$$dq = 2dk = \left(\frac{2}{a(k)}\right) \cdot d\varepsilon_k. \tag{62}$$

The integration for L_1 includes a partial integration in ε_k over the term containing the multiplier $(\partial^2 n_k / \partial \varepsilon_k^2)$, and after reducing it to an expression containing $(\partial n_k / \partial \varepsilon_k)$, the integration is finished by the use of eq. (6). The value of L obtained this way is substituted into the right hand side of eq. (20) giving the final result for σ as follows,

$$\sigma = \left(\frac{2e^2 V m_1^2}{9\pi^3 \hbar^5} \right) \left(\frac{m_1}{m_e} \right)^2 \left\{ \frac{1}{8k_f} \left(\frac{\partial |\mathbf{F}(k_f,q,k_f)|^2}{\partial q} \right)_{q=2k_f} + \frac{1}{4k_f} \left(\frac{\partial |\mathbf{F}(k,q,k_f)|^2}{\partial k} \right)_{\substack{k=k_f \\ q=2k_f}} + \frac{5}{16k_f^2} \left[1 - \frac{m_1}{m_2} \right] \left[|\mathbf{F}(k_f,q,k_f)|^2 \right]_{q=2k_f}$$

$$+\frac{1}{16k_f^4}\left[-1-4\frac{m_1}{m_2}+5\left(\frac{m_1}{m_2}\right)^2-2\frac{m_1}{m_3}\right]\int_0^{2k_f} dq\cdot q\cdot|\mathbf{F}(k_f,q,k_f)|^2$$

$$+\frac{1}{8k_f^3}\left[1-2\frac{m_1}{m_2}\right]\int_0^{2k_f} dq\cdot q\left(\frac{\partial|\mathbf{F}(k,q,k_f)|^2}{\partial k}\right)_{k=k_f}$$

$$+\frac{1}{16k_f^2}\int_0^{2k_f} dq\cdot q\left[2\left(\frac{\partial^2|\mathbf{F}(k,q,k_f)|^2}{\partial k^2}\right)_{k=kf}-\left(\frac{\partial^2|\mathbf{F}(k,q,k_1)|^2}{\partial k_1\partial k}\right)_{\substack{k=kf\\k1=kf}}\right]\Bigg\}, \tag{63}$$

where the obviously correct equations

$$\left(\frac{\partial|\mathbf{F}(k,q,k_1)|^2}{\partial k}\right)_{\substack{k=kf\\k1=kf}}=\left(\frac{\partial|\mathbf{F}(k,q,k_1)|^2}{\partial k_1}\right)_{\substack{k=kf\\k1=kf}}, \tag{64}$$

$$\left(\frac{\partial^2|\mathbf{F}(k,q,k_1)|^2}{\partial k^2}\right)_{\substack{k=kf\\k1=kf}}=\left(\frac{\partial^2|\mathbf{F}(k,q,k_1)|^2}{\partial k_1^2}\right)_{\substack{k=kf\\k1=kf}}, \tag{65}$$

have been applied.

This is the required formula for dc electrical conductivity σ of the considered isotropic model of conductors, in terms of the scattering matrix $|\mathbf{F}(k,q,k_1)|^2$, free of singularities, and with only one integration left to be performed afterwards, when the q dependence of the scattering matrix is explicitly given. The integration in k did not require explicit knowledge of the k dependence of the scattering matrix $|\mathbf{F}(k,q,k_1)|^2$, owing to the eq. (6), approximately valid for the assumed degenerate electronic gas of conductors.

2.3 Evaluation of the constitutive equation to σ calculation

The eq. (5) can be rewritten to the form

$$\alpha^*=1 \tag{66}$$

where

$$\alpha^*=\frac{1}{3Nm_e}\lim_{\omega\to0}\lim_{s\to+0}\int_{-\infty}^{0} dt\cdot(t)\cdot\cos(\omega t)e^{st}(\mathbf{F}(t);\mathbf{F}). \tag{67}$$

Substituting $(\mathbf{F}(t);\mathbf{F})$ by the right hand side of eq. (14), and then by integrating in t, from eq. (67) follows

$$\alpha^*=\left(\frac{\hbar^2}{6Nm_e}\right)\lim_{\omega\to0}\Bigg\{\lim_{s\to+0}\sum_{k,q}|<\Psi_{k+q}|\mathbf{F}|\Psi_k>|^2\left(\frac{n_k-n_{k+q}}{u}\right)$$

$$\left[\frac{1}{(u+\omega\hbar+i\hbar s)^2}+\frac{1}{(u+\omega\hbar-i\hbar s)^2}+\frac{1}{(u-\omega\hbar+i\hbar s)^2}+\frac{1}{(u-\omega\hbar-i\hbar s)^2}\right]\Bigg\}. \tag{68}$$

The two limits $(\omega\to0, s\to+0)$ are supposed to be performed by the formula [1, 15],

$$\lim_{\omega\to0}\lim_{s\to+0}\left(\frac{1}{(u\pm\omega\hbar+i\hbar s)^2}+\frac{1}{(u\pm\omega\hbar-i\hbar s)^2}\right)=\mathcal{V}.\mathcal{P}.\left(\frac{2}{u^2}\right), \tag{69}$$

where the label $\mathcal{V}.\mathcal{P}.$ has the meaning of the principal value taking. The symmetry in k and k_1, **($\mathbf{k}_1 = \mathbf{k} + \mathbf{q}$)**, of eq. (68) makes the multiplier $(n_k - n_{k+q})/u$ replaceable by the multiplier $(2n_k/u)$, and then after converting the summation in $\mathbf{k}$ and $\mathbf{q}$ into the integration in $\mathbf{k}$ and $\mathbf{q}$, eq. (68) for α^* reduces to

$$\alpha^* = \frac{8\hbar^2 V^2}{48\pi^4 N m_e}\mathcal{V}.\mathcal{P}.\int_0^{q_G} dq\cdot q^2 \int_0^{k_G} dk\cdot k^2 \cdot \int_0^{\pi} d\vartheta \sin(\vartheta)|\mathbf{F}(k,q,k_1)|^2 \left(\frac{n_k}{u^3}\right). \qquad (70)$$

The contours of integration in eqs.(19) and (70) are the same, however essential differences in the integrands, having root in the results of limits $(\omega \to 0, s \to +0)$ taken in the two formula, require different evaluation of these two formula. In the case of eq. (19) the mentioned limits resulted in some as narrow singular functions, peaked in $u = 0$, as δ function and its derivatives are, making possible to reduce the three-dimensional integrals into single-dimensional integrals, as it is seen in the result for σ given by eq. (63). In the case of eq. (70) the mentioned limits resulted in the function $\mathcal{V}.\mathcal{P}.(1/u^2)$, singular in the point $u = 0$, but this singularity is a broad function of u, and the dimension of integrations in eq. (70) cannot be lowered, under as general assumptions about the matrix element $| < \Psi_{k+q}|\mathbf{F}|\Psi_k > |^2$, as it is defined in eq. (17). In that sense, there is no possibility for any further evaluation of eq. (70).

3 Particular cases of $|\mathbf{F}(k,q,k_1)|^2$ and ε_k

3.1 Conductivity σ for the particular case of $|\mathbf{F}(k,q,k_1)|^2$

In this subsection, all properties of ε_k, as they are given at the start of subsection 2.1 are assumed kept, but $|\mathbf{F}(k,q,k_1)|^2$ is no longer assumed as general as it was in the preceding section. The dependence of $|\mathbf{F}(k,q,k_1)|^2$ on k and k_1, as defined by eqs. (11) and (17), does not come from the scattering Hamiltonian U, but from the Bloch functions $u_{k+q}(r)$ and $u_k(r)$ respectively. With Bloch functions approximated by plane waves, i.e. by putting $u_{k+q}(r) = 1$, $u_k(r) = 1$, the dependence of $|\mathbf{F}(k,q,k_1)|^2$ on k and k_1 disappears, implying the transition $|\mathbf{F}(k,q,k_1)|^2 \to |\mathbf{F}_q|^2$. We propose two ways of making this approximation, outlined in the subdivisions a) and b) as follow.

a.) The first one is direct. It emerges from eq. (11), when Bloch functions degenerate to plane waves giving

$$\mathbf{F}_q = -\frac{1}{V}\int_V d^3r \cdot e^{-i\mathbf{q}\cdot\mathbf{r}}\nabla_{\mathbf{r}}\left(U(r)\right), \qquad (71)$$

which after partial integration reads,

$$\mathbf{F}_q = -\frac{1}{V}\int_V d^3r \cdot \nabla_{\mathbf{r}}\left(e^{-i\mathbf{q}\cdot\mathbf{r}}U(r)\right) + \frac{1}{V}\int_V d^3r \cdot U(r)\nabla_{\mathbf{r}}\left(e^{-i\mathbf{q}\cdot\mathbf{r}}\right). \qquad (72)$$

Assuming the cyclic boundary conditions, the first integral on the right hand side of eq. (72) is zero, and we get

$$|\mathbf{F}_q|^2 = |\mathbf{q}|^2 \cdot |U_q|^2, \qquad (73)$$

where

$$U_q = \frac{1}{V}\int_V d^3r \cdot U(r)e^{-i\mathbf{q}\cdot\mathbf{r}}. \tag{74}$$

With this approximation for $|\mathbf{F}(k,q,k_1)|^2$, the eq. (63) for σ reduces to

$$\sigma = \left(\frac{e^2\pi V}{18\hbar k_f^2}\right)(N(\varepsilon_f))^2\left(\frac{m_1}{m_e}\right)^2(A + Z\cdot B + Z_3\cdot C), \tag{75}$$

where

$$A = \left[\frac{\partial|U_Q|^2}{\partial Q}\right]_{Q=1}, \tag{76}$$

$$B = \left[|U_Q|^2\right]_{Q=1}, \tag{77}$$

$$C = \int_0^1 dQ.Q^3|U_Q|^2, \tag{78}$$

$$Z = \left(7 - 5\frac{m_1}{m_2}\right), \tag{79}$$

$$Z_3 = 4\left(-1 - 4\frac{m_1}{m_2} + 5\left(\frac{m_1}{m_2}\right)^2 - 2\frac{m_1}{m_3}\right). \tag{80}$$

In eqs. (76) - (78), the wavenumber q has been substituted by the dimensionless wavenumber Q defined by

$$Q = \left(\frac{q}{2k_f}\right), \tag{81}$$

and the density of states at Fermi surface $N(\varepsilon_f)$ has been introduced into eq. (75), where $N(\varepsilon_f)$, with spin degeneration included [17], reads

$$N(\varepsilon_f) = \left(\frac{k_f^2}{\pi^2(\partial\varepsilon_k/\partial k)_f}\right) = \left(\frac{k_f m_1}{\pi^2\hbar^2}\right). \tag{82}$$

b.) The second way of approximating eq. (63), is based on the relation $\mathbf{F} = (1/i\hbar)[\mathbf{P}, U]$ implying

$$\begin{aligned} <\Psi_{k1}|\mathbf{F}|\Psi_k> = \frac{1}{i\hbar}\sum_{k_2}(&<\Psi_{k1}|\mathbf{P}|\Psi_{k2}><\Psi_{k2}|U|\Psi_k> \\ &- <\Psi_{k1}|U|\Psi_{k2}><\Psi_{k2}|\mathbf{P}|\Psi_k>), \end{aligned} \tag{83}$$

and since Ψ_k are eigenfunctions of H_0, and $\mathbf{P}$ commutes with H_0 (see eq. (9) and the discussion preceding it), $\mathbf{P}$ is diagonal in this representation, therefore $< \Psi_{k1}|\mathbf{P}|\Psi_{k2} >= \delta_{k1,k2} \cdot < \Psi_{k1}|\mathbf{P}|\Psi_{k1} >, < \Psi_{k2}|\mathbf{P}|\Psi_k >= \delta_{k2,k} \cdot < \Psi_k|\mathbf{P}|\Psi_k >$, with

$$< \Psi_{k1}|\mathbf{P}|\Psi_{k1} >= \frac{m_e}{m_1}\hbar\mathbf{k}_1 = \frac{m_e}{m_1}\hbar(\mathbf{k}+\mathbf{q}), \tag{84}$$

$$< \Psi_k|\mathbf{P}|\Psi_k >= \frac{m_e}{m_1}\hbar\mathbf{k}, \tag{85}$$

where m_1 is defined in eq. (55). With the matrix elements of the momentum $\mathbf{P}$, as they are given here, eq. (83) reads,

$$< \Psi_{k1}|\mathbf{F}|\Psi_k >= -i < \Psi_{k1}|U|\Psi_k > (\frac{m_e}{m_1})q. \tag{86}$$

After the Bloch functions in $< \Psi_{k1}|U|\Psi_k >$ are replaced by plane waves, from eq. (86) follows,

$$|\mathbf{F}_q|^2 = \left(\frac{m_e}{m_1}\right)^2 |U_q|^2 q^2. \tag{87}$$

Instead of approximating $< \Psi_{k+q}|\mathbf{F}|\Psi_k >$, like we have done it in obtaining eq. (73), here we have approximated $< \Psi_{k+q}|U|\Psi_k >$, and we have obtained a result which is different from the preceding one, but only in the case when $m_e \neq m_1$, i.e. when the velocity mass m_1 as it is modified by the coupling of carriers to the periodic potential, is different from the free electronic mass m_e. Here, instead of eq. (75), for σ we have,

$$\sigma = \left(\frac{e^2\pi V}{18\hbar k_f^2}\right)(N(\varepsilon_f))^2[A + Z \cdot B + Z_3 \cdot C]. \tag{88}$$

Which one of the two expressions, eq. (75) or eq. (88) is the better approximation for eq. (63), hardly can be decided solely from the theoretical arguments.

3.2 Case of ε_k parabolic in k dependence

For the particular case, when the scattering matrix is $|\mathbf{F}_q|^2$, k and k_1 independent, and in addition the energy ε_k is parabolic in k,

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m_1}, \tag{89}$$

with m_1 as a constant effective carrier mass, there is no need for eq. (6) to be applied in order to obtain a tractable expressions for σ in the framework of our concept, as we are going to see it in this subsection.

In this particular case, σ is calculated by eq. (20) and (21), but L, $J(q)$ and $I(k,q)$ are no longer calculated by eqs. (22) - (24), instead they are calculated as follow

$$L = \left(\frac{2m_1}{\hbar^2}\right)\int_0^{q_G} dq \cdot q \cdot |\mathbf{F}_q|^2 \cdot J(q), \tag{90}$$

$$J(q) = \int_0^{k_G} dk \cdot k \cdot I(k,q), \tag{91}$$

$$I(k,q) = \int_{u_D}^{u_G} du \cdot \left(\frac{n_k - n_{k+q}}{u}\right) \frac{\partial^2(\delta(u))}{\partial u^2}, \tag{92}$$

where

$$u_D = (\hbar^2/2m_1)q(q-2k), \tag{93}$$

$$u_G = (\hbar^2/2m_1)q(q+2k). \tag{94}$$

By double partial integration in u, from eq. (92) follows,

$$I(k,q) = I_2(k,q) + I_1(k,q) + I_0(k,q), \tag{95}$$

$$I_2(k,q) = \left\{ (\frac{n_k - n_{k+q}}{u}) \cdot \frac{\partial(\delta(u))}{\partial u} \right\}\Big|_{u_D}^{u_G}, \tag{96}$$

$$I_1(k,q) = -\left\{ \frac{\partial}{\partial u}(\frac{n_k - n_{k+q}}{u}) \cdot \delta(u) \right\}\Big|_{u_D}^{u_G}, \tag{97}$$

$$I_0(k,q) = \int_{u_D}^{u_G} du \cdot \frac{\partial^2}{\partial u^2}(\frac{n_k - n_{k+q}}{u}) \cdot \delta(u). \tag{98}$$

The integration in eq. (98), by making use of eq. (119) results in

$$I_0(k,q) = (\frac{-1}{3}) \left(\frac{\partial^3 n_k}{\partial \varepsilon_k^3}\right) \cdot \Theta(-u_D) \cdot \Theta(u_G), \tag{99}$$

where $\Theta(-u_D)$ and $\Theta(u_G)$ are the Heaviside's step functions. By substituting right hand side of eq. (99) into eq. (91) we obtain $J_0(q)$, the contribution of $I_0(k,q)$ to $J(q)$,

$$J_0(q) = (\frac{-1}{3}) \int_{(q/2)}^{k_G} dk \cdot k \cdot (\frac{\partial^3 n_k}{\partial \varepsilon_k^3}), \tag{100}$$

and after performing the integration in k resulting in

$$J_0(q) = (\frac{m_1}{3\hbar^2}) \left(\frac{\partial^2 n_k}{\partial \varepsilon_k^2}\right)_{k=q/2}. \tag{101}$$

The contribution of $I_1(k,q)$ to $J(q)$, denoted by $J_1(q)$, from eqs. (97) and (91) results in

$$J_1(q) = (\frac{-m_1}{4\hbar^2}) \cdot \left(\frac{\partial^2 n_k}{\partial \varepsilon_k^2}\right)_{k=q/2}, \tag{102}$$

while the contribution of $I_2(k,q)$ to $J(q)$ is zero, therefore $J(q) = J_0(q) + J_1(q)$, leading by eqs. (20) and (90) to the result for σ,

$$\sigma = (\frac{Ve^2}{48 \cdot 6\pi^3\hbar})(\frac{m_1}{m_e})^2 \int_0^{q_G} dq \cdot q \cdot |\mathbf{F}_q|^2 \cdot \left(\frac{\partial^2 n_k}{\partial \varepsilon_k^2}\right)_{k=q/2}. \tag{103}$$

The eq. (70) for α^*, in this particular case can be reduced to an expression giving α^* in terms of a double-dimensional integral,

$$\alpha^* = \frac{V^2 m_1^2}{3\pi^4 \hbar^4 N} \left(\frac{m_1}{m_e}\right) \mathcal{V}.\mathcal{P}. \int_0^{q_G} dq \cdot q^{-1} \cdot |\mathbf{F}_q|^2 \int_0^{k_G} dk \cdot k^1 \cdot n_k \left[\frac{1}{(q-2k)^2} - \frac{1}{(q+2k)^2}\right]. \tag{104}$$

In obtaining eq. (104), the integration in ϑ has been substituted by the integration in u, by making use of eqs. (15) and (89), which give: $\sin(\vartheta)d\vartheta = (-m_1/\hbar^2 kq)du$, and the integration in u has been carried out easily afterwards.

Two approximate formula for $|\mathbf{F}_q|^2$ have been derived in the preceding section, given by eqs. (73) and (87) respectively. By substituting $|\mathbf{F}_q|^2$ with the right hand side of eq. (73), from eq.(103) follows

$$\sigma = (\frac{Ve^2}{48 \cdot 6\pi^3 \hbar})(\frac{m_1}{m_e})^2 \int_0^{q_G} dq \cdot q^3 \cdot |U_q|^2 \cdot \left(\frac{\partial^2 n_k}{\partial \varepsilon_k^2}\right)_{k=q/2}, \tag{105}$$

and from eq. (104) for α^* follows:

$$\alpha^* = \frac{V^2 m_1^2}{3\pi^4 \hbar^4 N} \left(\frac{m_1}{m_e}\right) \mathcal{V}.\mathcal{P}. \int_0^{q_G} dq \cdot q \cdot |U_q|^2 \int_0^{k_G} dk \cdot k \cdot n_k \left[\frac{1}{(q-2k)^2} - \frac{1}{(q+2k)^2}\right], \tag{106}$$

while from substitution of $|\mathbf{F}_q|^2$ with the right hand side of eq. (87) for σ follows

$$\sigma = (\frac{Ve^2}{48 \cdot 6\pi^3 \hbar}) \int_0^{q_G} dq \cdot q^3 \cdot |U_q|^2 \cdot \left(\frac{\partial^2 n_k}{\partial \varepsilon_k^2}\right)_{k=q/2}, \tag{107}$$

and for α^* follows

$$\alpha^* = \frac{V^2 m_1^2}{3\pi^4 \hbar^4 N} \left(\frac{m_e}{m_1}\right) \mathcal{V}.\mathcal{P}. \int_0^{q_G} dq \cdot q \cdot |U_q|^2 \int_0^{k_G} dk \cdot k \cdot n_k \left[\frac{1}{(q-2k)^2} - \frac{1}{(q+2k)^2}\right]. \tag{108}$$

Like in the preceding section, here it is not easy to conclude which choice for $|\mathbf{F}_q|^2$ is the better approximation.

If the eq. (6) is applied additionally to eqs. (105) and (107) the eqs. (75) and (88) follow respectively.

4 Discussion and Conclusions

The first item to be discussed here is how σ given by eq. (75) or eq. (88) behaves with $V \to \infty$, where V is the volume of the system. The integral in eq. (74) is the Fourier transform of $U(\mathbf{r})$, of a function having random (stochastic) dependence on $\mathbf{r}$, like it has been outlined in

connection with eqs. (8) - (10). For such $U(\mathbf{r})$ it has been shown [11] that the square of the integral's module in eq. (74) is proportional to V,

$$\left| \int_V d^3r \cdot U(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \right|^2 \sim V, \tag{109}$$

and from eqs. (74) and (109) follows $|U_q|^2 \sim V^{-1}$, and corresponding to eqs. (76) - (78), $A \sim V^{-1}$, $B \sim V^{-1}$, $C \sim V^{-1}$, and finally from eq. (75) or eq. (88) we conclude that σ is a certain quantity independent of V in the limit $V \to \infty$, as it should be.

The second item deserving a discussion is the impact to σ and α^* calculation, of the double limits ($\omega \to 0$, $s \to +0$). In the case of σ, the double limits resulted in a δ-function of u, meaning that σ has got non-zero contribution only from the processes where the energy conservation law in the scattering is fulfilled, i.e. where $u = 0$. The energy conservation law exerts clearly pronounced restrictive role here. In the formula for α^* the mentioned limits resulted in $\mathcal{V}.\mathcal{P}.(1/u^2)$, meaning that α^* has got non-zero contributions also from the processes where the energy conservation law in scattering is not fulfilled, where $u \neq 0$. Therefore, the restrictive role of the energy conservation law is missing here. The physics of this differences is to be looked for in the fact that α^* relates the non-dissipative component of the current [1].

The third item to be mentioned here is the σ dependence on the carriers density of states $N(\varepsilon_f)$, which appears to be squared in $N(\varepsilon_f)$, as it is given in eqs. (75) and (88). A result resembling ours in that respect, has been obtained by Mott and Davis [17] (see formula (2.14) in Ref. [17]). However, full comparison of our result to the mentioned results in [17] is impossible, since the term $|D_E|^2_{av}$ in [17] has been loosely defined, and not accounted for effectively by means of the linear response theory, but instead only globally interpreted in terms of the relaxation time τ. We ascertain, the linear response theory of dc electrical transport, as applied in [17], was not performed consequently, instead it was abandoned when the most delicate step, the calculation of $|D_E|^2_{av}$ came in turn. Unlike it, the aim of the present work is to apply the means of the linear response theory as consequent as possible.

In cases of ac electrical conduction, with very high external driving frequencies ω, like the optical frequencies are, the linear response formula (Kubo formula) for conductivity $\sigma(\omega)$ has got proof in practice, but it is not the case with the low frequencies, and certainly not with the dc current. The reason for this state of art is not clear yet, and the discussion on this subject is still running on [2, 4]. We assume that the linear response formula though correct, is not enough by itself to give a correct description of the conductivity, but it can fulfill its role in conjunction with some constitutive equations, like eqs.(106) or (108) are. The constitutive equation provides information about the alteration of the system's parameters taking place in the system while the dc current is running in it, that way having impact on the dc conductivity. Detailed demonstration of the calculation of σ in conjunction with the constitutive equation, will be given in the third part of this work.

Appendix

We first evolve the right hand side of eq. (32) to the form:

$$\left\{\frac{\partial^2}{\partial u^2}\left[D(k,q,k_1)\left(\frac{n_k-n_{k+q}}{u}\right)\right]\right\}_{u=0}=D_1(k,q,k_1)\left(\frac{n_k-n_{k+q}}{u}\right)_{u=0}$$
$$+2D_2(k,q,k_1)\left\{\frac{\partial}{\partial u}\left(\frac{n_k-n_{k+q}}{u}\right)\right\}_{u=0}+3D_3(k,q,k_1)\left\{\frac{\partial^2}{\partial u^2}\left(\frac{n_k-n_{k+q}}{u}\right)\right\}_{u=0}, \tag{110}$$

$$D_1(k,q,k_1)=\left\{\frac{\partial^2}{\partial u^2}D(k,q,k_1)\right\}_{u=0}, \tag{111}$$

$$D_2(k,q,k_1)=\left\{\frac{\partial}{\partial u}D(k,q,k_1)\right\}_{u=0}, \tag{112}$$

$$D_3(k,q,k_1)=\left(\frac{1}{3}\right)\left(D(k,q,k_1)\right)_{u=0}, \tag{113}$$

where $D(k,q,k_1)$ is defined by eq. (27). The problem we are faced with here, is how to determine the above derivatives in u, taken for $u=0$. From Fig. 1. we see that the vector $\mathbf{k}$ and the length of vector $\mathbf{q}$ are kept constant, when the top of vector $\mathbf{k_1}$ moves on the semicircle of the integration in u, and the aforementioned derivative in u, due to eq. (15), can be replaced by the derivative in ε_{k_1} ($k_1=|\mathbf{k}+\mathbf{q}|$):

$$\frac{\partial D(k,q,k_1)}{\partial u}=\frac{\partial D(k,q,k_1)}{\partial \varepsilon_{k1}}. \tag{114}$$

The subsequent taking of $u=0$ is equivalent to taking equal vector lengths, $k=k_1$. In this *Appendix*, as well as in the main body of this article, the differential operator $(\partial/\partial\varepsilon_{k1})$ or $(\partial/\partial\varepsilon_k)$, appears a number of times. It always operates by the formula :

$$\frac{\partial}{\partial\varepsilon_{k1}}=\left(\frac{\partial\varepsilon_{k1}}{\partial k_1}\right)^{-1}\frac{\partial}{\partial k_1}. \tag{115}$$

In this way, from eqs. (111) - (113), the eqs. (35) - (37) for $D_1(k,q,k_1)$, $D_2(k,q,k_1)$ and $D_3(k,q,k_1)$ follow respectively.

By applying the series expansion in u to n_{k+q} :

$$n_{k+q}=n_k+\left(\frac{\partial n_k}{\partial\varepsilon_k}\right)u+\left(\frac{1}{2}\right)\left(\frac{\partial^2 n_k}{\partial\varepsilon_k^2}\right)u^2+\left(\frac{1}{6}\right)\left(\frac{\partial^3 n_k}{\partial\varepsilon_k^3}\right)u^3+..., \tag{116}$$

the following relations are easily derived :

$$\left(\frac{n_k-n_{k+q}}{u}\right)_{u=0}=\left(\frac{-\partial n_k}{\partial\varepsilon_k}\right), \tag{117}$$

$$\left\{\frac{\partial}{\partial u}\left(\frac{n_k-n_{k+q}}{u}\right)\right\}_{u=0}=\left(\frac{1}{2}\right)\left(\frac{-\partial^2 n_k}{\partial\varepsilon_k^2}\right), \tag{118}$$

$$\left\{\frac{\partial^2}{\partial u^2}\left(\frac{n_k - n_{k+q}}{u}\right)\right\}_{u=0} = \left(\frac{1}{3}\right)\left(\frac{-\partial^3 n_k}{\partial \varepsilon_k^3}\right). \tag{119}$$

By inserting right hand sides of eqs. (117) - (119) into eq. (110), the required eq. (33) for $I_0^*(k,q)$ is obtained.

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