Low-frequency plasma conductivity in the average-atom approximation

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Low-frequency properties of a plasma are examined within the average-atom approximation, which presumes that scattering of a conducting electron on each atom takes place independently of other atoms. The relaxation time τ distinguishes a high-frequency region $\omega\tau>1$, where the single-atom approximation is applicable explicitly, from extreme low frequencies $\omega\tau<1$, where, naively, the single-atom approximation is invalid. A proposed generalization of the formalism, which takes into account many-atom collisions, is found to be accurate in all frequency regions, from $\omega=0$ to $\omega\tau>1$, reproducing the Ziman formula in the static limit, results based on the Kubo-Greenwood formula for high frequencies and satisfying the conductivity sum rule precisely. The correspondence between physical processes leading to the conventional Ohm's law and the infrared properties of QED is discussed. The suggested average-atom approach to frequency-dependent conductivity is illustrated by numerical calculations for an aluminum plasma in the temperature range 2–10 eV.

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I. INTRODUCTION

Various theoretical approaches are available to investigate the frequency-dependent conductivity of plasmas, ranging from methods based on a many-body expansion of the grand canonical partition function [1–3] to methods based on molecular dynamics simulations [4–9]. In the present paper, we reexamine an average-atom approach [10] that has been used to investigate anomalous dispersion in C, Al, Ag, and other plasmas in the soft x-ray region (14–47 nm) of the spectrum [11–15]. Clérouin *et al.* [16] have recently compared results from the average-atom model with simulations on hot expanded boron. The model's utility rests on its simplicity and wide range of applicability.

At low frequencies, electron-ion scattering contributions dominate the conductivity $\sigma(\omega)$, while at higher frequencies (e.g., in the x-ray region mentioned above) photoionization and bound-bound transitions provide the most important contributions. Effects of multiple scattering were omitted in evaluating free-free contributions to $\sigma(\omega)$ in Ref. [10], leading to a (spurious) second-order pole at $\omega=0$, which was regularized in an *ad hoc* way. In the paragraphs below, we discuss the origin of this pole in more detail and give a modified formula for the free-free contribution to $\sigma(\omega)$ that accounts for multiple scattering, is regular at $\omega=0$, and rigorously satisfies the conductivity sum rule.

The present discussion concerns the plasma conductivity $\sigma(\omega)$ at low frequencies—i.e., presuming that the frequency ω is lower than both the plasma frequency and typical frequencies of atomic excitations:

$$\omega \ll (4\pi n_e e^2/m)^{1/2}, \quad me^4/\hbar^3. \tag{1.1}$$

The only parameter that drives the conductivity in this region is the relaxation time τ, which establishes a boundary between relatively high frequencies $\omega\tau>1$, which will be called the *high frequencies* for short, and extreme low frequencies, where $\omega\tau<1$ including the static limit $\omega=0$; these frequencies will be called the *ultralow frequencies*.

Physical processes, which govern the conductivity in these two regions, differ qualitatively, as discussed in detail below. Alongside this physical difference, there exists also a distinction in theoretical methods. One line of research is based on the Ziman formula, which is applicable in the static limit, leading to the conventional static Ohm's law; see Ziman [17], Chap. 7, and Mahan [18], Chap. 8. An alternative approach is based on the Kubo-Greenwood formula [19–23], which usually gives a reliable description of conductivities at high frequencies.

Generally speaking, the Kubo-Greenwood formalism should lead to accurate results for arbitrary frequencies, provided though that all *important* scattering processes are taken into account. However, typically, within some given theoretical scheme, it is feasible to account only for some particular class of scattering events. This restriction may substantially reduce an area of applicability for the Kubo-Greenwood formalism. In particular, it is usually difficult to extend its validity to the static limit. An example illustrating the latter fact is provided by models based on the average-atom approximation. In such models, scattering of conducting electrons is assumed to take place on each atom, independently of other atoms. This means that many-atom events (multiple scattering), in which several atoms produce a coherent contribution, are neglected. The simplicity and clear physical nature of the average-atom approximation make it popular. Its origins can be traced to the Thomas-Fermi model of plasma devised more than a half century ago by Feynman, Metropolis, and Teller [24]. A quantum mechanical version of the average-atom model is given by Blenski and Ishikawa [25], and a recent implementation is found in Ref. [10].

The present work shows that scattering processes which take place at ultralow frequencies necessarily include several atoms. We will call these processes *many-atom* collisions for

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short. Their importance indicates that for ultra low frequencies the single-atom approximation breaks down. This fact explains a difficulty that occurs in the Kubo-Greenwood formalism in the static limit. The breakdown of the single-atom approximation manifests itself as a divergence of the conductivity calculated in the Kubo-Greenwood formalism in the limit $\omega \to 0$. As mentioned in the Introduction, the conductivity in this limit exhibits a second-order pole.

Thus, direct numerical calculations based on an average-atom approximation and relying on the Kubo-Greenwood approach are applicable for high frequencies only, while for lower frequencies, where the many-atom collisions are important, the formalism faces a difficulty. This work resolves this difficulty, proposing an approach that is applicable for frequencies that satisfy the inequality (1.1). In the static limit $\omega=0$, our description reproduces the Ziman formula. For high frequencies $\omega\tau > 1$, our results agree with the conventional Kubo-Greenwood description. In the intermediate region $\omega\tau \simeq 1$, the validity of our formalism is supported by the fact that it provides the correct result for the conductivity sum rule. One of the important advantages of the proposed description is related to its simplicity. We show that all necessary physical quantities can be evaluated using a simple single-atom approximation. This means that multiple scattering, which is paramount in the static limit, is accounted for effectively in the single-atom approximation.

There is an important relation between the divergence in the conductivity at ultralow frequencies and the infrared problem of quantum electrodynamics (QED). To make this point more transparent, let us keep in mind that the conductivity describes absorption and emission of quanta of the electromagnetic field, which are possible due to electron scattering. Presuming that the potential, which is responsible for scattering, is localized in a vicinity of some atom, one can express the amplitude of absorption, $f_{\rm abs}$ (or emission), in terms of the elastic scattering amplitude f. This relation reveals that the absorption amplitude has a pole at $\omega=0$

$$f_{\rm abs} \propto \frac{f}{\omega}, \quad \omega \to 0. \tag{1.2}$$

This general, well-known, feature of the infrared processes in QED is described by Feynman diagrams with a photon line inserted into the outer electron legs as is shown in Fig. 1. The first-order pole in the absorption amplitude in Eq. (1.2) leads to a second-order pole in the conductivity:

$$\sigma(\omega) \propto \frac{1}{\omega^2}. \tag{1.3}$$

Developing this argument, we will show below that many-atom collisions prevent the divergence of the scattering amplitude in Eq. (1.2) at $\omega \to 0$. This happens because many-atom collisions lead to a finite relaxation time τ, which measures the interval of time during which the electron travels between two subsequent collisions with different atoms. We show that the relaxation time provides an effective cutoff for the amplitude in Eq. (1.2), in which the pole is replaced by a finite quantity $|f_{\rm abs}| \simeq 1/\omega_{\rm min} = \tau$. The well-defined, finite, scattering amplitude leads to a conductivity that is regular at $\omega=0$; Eq. (1.3) is replaced by the relation $\sigma(\omega) \propto 1/\omega_{\rm min}^2 = \tau^2$.

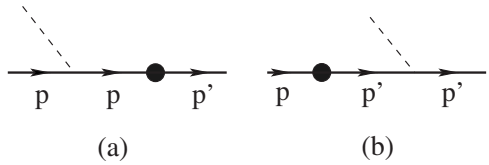

FIG. 1. Two Feynman diagrams represent the amplitude, which describes electron scattering with absorption of a quantum of the electromagnetic field, which has frequency ω and small wave vector that leaves the electron momentum unchanged. The solid lines show the electron propagation, the dashed line the quantum of the electromagnetic field, and the solid circles the elastic scattering process. In diagrams (a) and (b) the lines that represent the electromagnetic quantum are inserted into the outer legs, which makes these diagrams infrared singular, $\propto 1/\omega$, when $\omega \to 0$. Other possible diagrams have no such singularity.

Our discussion below presumes that the plasma conductivity is due mainly to scattering of conducting electrons by atomic cores. There exist other mechanisms contributing to conductivity. One of them is related to electron-electron scattering. The main idea of this work can be generalized to cover this mechanism (and others) as well. However, in order to keep our presentation simple and clear, we will not attempt to formulate the idea in the most general case, restricting our discussion to electron-atom scattering only. At sufficiently high temperatures, when atomic cores are highly ionized, one expects that electron-atom scattering gives the dominant contribution to the conductivity owing to the fact that scattering by an ion is a coherent process, with probability proportional to $Z_{\rm ion}^2$, where $Z_{\rm ion}$ is the ionic charge. By contrast, electron-electron scattering is an incoherent process with probability proportional to $Z_{\rm ion}$. Thus, scattering by an ion is expected to dominate electron-electron scattering, provided $Z_{\rm ion} > 1$.

II. SINGLE-ATOM APPROXIMATION FOR HIGH FREQUENCIES

A. Absorption of photons and elastic scattering

We need to recall several simple important facts related to absorption of low-frequency quanta by electrons. Let us presume that there is a localized potential $U=U(\mathrm{r})$, which causes electron scattering. Let us assume further that there is some external low-frequency homogeneous electric field. [26] Then scattering can be accompanied by absorption of a quantum of the electromagnetic field. The process of absorption is described by the matrix element $f_{\rm abs}$:

$$f_{\rm abs} = \langle \psi_f | \boldsymbol{\epsilon} \cdot \boldsymbol{p} | \psi_i \rangle. \tag{2.1}$$

Here $\boldsymbol{\epsilon}$ and $\mathbf{p}$ are the polarization vector of the electromagnetic quantum and the operator of momentum of the electron, and ψ_i and ψ_f are the wave functions of the electron in the initial and final states. We are interested in the low-frequency region specified by Eq. (1.1). Our first goal is to simplify the matrix element in Eq. (2.1), presenting it as

$$f_{\rm abs} = \frac{\boldsymbol{\epsilon}\cdot\boldsymbol{p}}{\hbar\omega}\langle\psi_{\mathbf{p}'}|U|\mathbf{p}\rangle - \frac{\boldsymbol{\epsilon}\cdot\mathbf{p}'}{\hbar\omega}\langle\mathbf{p}'|U|\psi_{\mathbf{p}}\rangle. \tag{2.2}$$

Here the first and second terms correspond to the Feynman diagrams, in which the line representing the electromagnetic quantum is inserted into the left and right legs of the diagram respectively; see Fig. 1. The wave functions $|\mathbf{p}\rangle$ and $|\psi_{\mathbf{p}}\rangle$ in Eq. (2.2) describe the electron propagation in the plane-wave approximation and with account of the potential U, respectively. All processes, in which the line representing the electromagnetic quantum is inserted into internal parts of the diagram, have no poles in the limit $\omega\to 0$, allowing one to neglect them in Eq. (2.2) [see the more detailed discussion after Eq. (2.4)].

Generally speaking, the electron energy in the initial and final states of the photoabsorption process are different. However, for low frequencies this difference is insignificant. Neglecting it, one can presume that the matrix elements in Eq. (2.2) are related to elastic events—i.e., $|\mathbf{p}|=|\mathbf{p}'|$. Remember now that the elastic scattering amplitude is defined as

$$f = -\frac{m}{2\pi\hbar^2}\langle\psi_{\mathbf{p}'}|U|\mathbf{p}\rangle = -\frac{m}{2\pi\hbar^2}\langle\mathbf{p}'|U|\psi_{\mathbf{p}}\rangle. \tag{2.3}$$

Consequently one finds from Eq. (2.2) that

$$f_{\rm abs} = \frac{2\pi\hbar}{m\omega}(\boldsymbol{\epsilon}\cdot\mathbf{q})f, \tag{2.4}$$

where $\mathbf{q}=\mathbf{p}'-\mathbf{p}$ is the transferred momentum.

Equation (2.4) relates the amplitude of the process with absorption of a low-frequency electromagnetic quantum and the amplitude of elastic scattering [compare Eq. (1.2)]. Relations of this type provide a basis for the known infrared problem in QED; see, e.g., [27]. Figure 1 can be considered as a diagrammatic representation of Eq. (2.4). The singular energy denominator $1/\omega$, which appears in Eq. (2.4), arises only in the external legs of the two Feynman diagrams shown in this picture. All energy denominators of all other diagrams include virtual energies of the atomic excitations, which are sufficiently high compared with the energy of the electromagnetic quantum. Correspondingly, all other diagrams, which are not shown in Fig. 1, are all finite in the limit $\omega\to 0$. This fact distinguishes the two diagrams in Fig. 1 and guarantees that Eq. (2.4) is accurate for low frequencies.

From Eq. (2.1) one finds

$$|f_{\rm abs}|^2 = \left(\frac{2\pi\hbar}{m\omega}\right)^2(\boldsymbol{\epsilon}\cdot\boldsymbol{q})^2|f|^2. \tag{2.5}$$

Averaging over possible orientations of the polarization vector one writes

$$\langle(\boldsymbol{\epsilon}\cdot\boldsymbol{q})^2\rangle = \frac{1}{3}q^2 = \frac{2}{3}(1-\cos\theta)p^2, \tag{2.6}$$

where the angular brackets $\langle\cdots\rangle$ refer to the averaging procedure and θ is the scattering angle. Equations (2.5) and (2.6) give

$$\int\langle|f_{\rm abs}|^2\rangle d\Omega = \frac{2}{3}\left(\frac{2\pi\hbar p}{m\omega}\right)^2\int(1-\cos\theta)|f|^2 d\Omega, \tag{2.7}$$

where the integration runs over the angles Ω of the scattered electron. The factor

$$\sigma_{\rm tr} = \int(1-\cos\theta)|f|^2 d\Omega \tag{2.8}$$

represents the transport cross section on the potential U. Equations (2.7) and (2.8) give

$$\int\langle|f_{\rm abs}|^2\rangle d\Omega = \frac{2}{3}\left(\frac{2\pi\hbar v}{\omega}\right)^2\sigma_{\rm tr}. \tag{2.9}$$

Here $v=p/m$ is the velocity of the electron. The quantity on the left-hand side of Eq. (2.9) describes the probability of absorption of low-frequency quanta. The transport cross section on the right-hand side is related to elastic scattering. A close connection between low-frequency electromagnetic processes and elastic scattering is well known; see, e.g., Ref. [27].

Deriving Eq. (2.9), we assumed that the potential U responsible for the electron scattering is localized within some finite volume. Precisely this property allows one to distinguish the two Feynman diagrams in Fig. 1. Otherwise, if the potential is spread all over an infinite volume, a mere concept of an external leg of the diagram would make no sense.

We can specify the potential U assuming that it is created by a single atom. In that case Eq. (2.9) describes those events that take place during electron scattering by a single atom, being thus closely related to the single-atom approximation.

B. Kubo-Greenwood formalism

Consider the conductivity of plasma, which is due to scattering of conducting electrons by atoms. Within the Kubo-Greenwood formalism it can be written as

$$\sigma(\omega) = \frac{2\pi n_{\rm a}e^2}{\omega}\int|\langle\psi_{p'}|\boldsymbol{\epsilon}\cdot\boldsymbol{v}|\psi_p\rangle|^2(\mathsf{f}_p-\mathsf{f}_{p'}) \times\delta(E_p-E_{p'}-\omega)\frac{d^3p}{(2\pi\hbar)^3}\frac{d^3p'}{(2\pi\hbar)^3}, \tag{2.10}$$

where $n_{\rm a}$ is the density of atoms and f_p is the Fermi distribution function for conducting electrons (which will be denoted by f below):

$$\mathsf{f}_p = \frac{1}{\exp[(E_p-\mu)/kT]+1}. \tag{2.11}$$

The chemical potential μ here is related to the concentration of conducting electrons $n_{\rm c}$:

$$2\int\mathsf{f}\frac{d^3p}{(2\pi\hbar)^3} = n_{\rm c}, \tag{2.12}$$

where the coefficient 2 accounts for two projections of spin. It should be noted that we have omitted contributions to Eq. (2.10) arising from atomic bound states. These contributions, which lead to bound-bound resonances and singularities near

photoionization thresholds, are insignificant in the low-frequency region of concern herein.

The first factor in the integrand in Eq. (2.10) can be conveniently rewritten with the help of Eqs. (2.1) and (2.9); the difference of the distribution functions in the integrand can be simplified using the low-frequency approximation. These transformations allow one to simplify the expression for conductivity, Eq. (2.10), reducing it to

$$\sigma(\omega) = \frac{2}{3}\frac{n_a e^2}{\omega^2}\int v^3 \sigma_{tr}\left(-\frac{\partial f}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}. \tag{2.13}$$

It is convenient to introduce the relaxation time τ_p for conducting electrons, which is due to collisions with atoms:

$$\tau_p = \frac{1}{v n_a \sigma_{tr}}. \tag{2.14}$$

Clearly, it depends on the electron momentum via the velocity and the transport cross section. Equation (2.13) can be written in this notation in a transparent compact form

$$\sigma(\omega) = \frac{2e^2}{3}\int \frac{v^2}{\omega^2 \tau_p}\left(-\frac{\partial f}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}. \tag{2.15}$$

This is, in fact, the low-frequency limit of the Kubo-Greenwood formula in the single-atom approximation.

There are two conditions that restrict a region of frequencies in which Eq. (2.15) is valid. First, as was mentioned, the frequency must be sufficiently low. More precisely, this condition implies that the relevant scattering phases $\delta_l(E)$, where l is a typical orbital momentum, should not reveal significant variation in the interval of frequencies ω:

$$\hbar\omega\left|\frac{d\delta_l(E)}{dE}\right| \ll 1. \tag{2.16}$$

Here E is a typical energy of conducting electrons. Second, the frequency is restricted from below by

$$\omega\tau_p > 1, \tag{2.17}$$

$\boldsymbol{p}$ being a typical momentum of those electrons that give significant contributions to the conductivity in Eq. (2.15). We will discuss this condition in detail after Eq. (4.8). Here, let us mention briefly that the necessary high frequency specified by Eq. (2.17) makes it certain that scattering processes on different atoms take place incoherently, as independent events—in other words, that the single-atom approximation is valid. Equation (2.15) predicts a simple $\propto 1/\omega^2$ behavior of the conductivity on frequency. If one ignores the restriction given in Eq. (2.17) by taking the static limit in Eq. (2.15) naively, then this equation clearly indicates that the conductivity has a second-order pole at $\omega=0$, as seen in Eq. (1.3). Figure 2 illustrates this statement by comparing calculations based on the complete Kubo-Greenwood formula, Eq. (2.10), with predictions of Eq. (2.15). As an example, an aluminum plasma at temperature of 5 eV was taken in Fig. 2. The agreement between the two sets of calculations, shown as the solid and dashed lines in Fig. 2, supports the validity of the approximations, which led to Eq. (2.15). The numerical code for calculations reported in the present work is based on the an earlier average-atom Kubo-Greenwood conductivity code given in Ref. [10], where the divergence at $\omega=0$ was removed in an *ad hoc* manner.

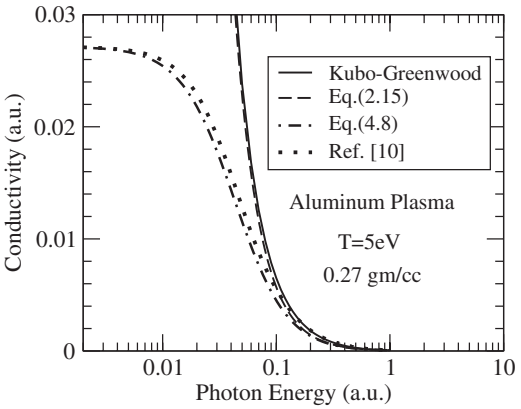

FIG. 2. The conductivity of an aluminum plasma at $T=5$ eV. Solid line, the Kubo-Greenwood formula, Eq. (2.10). Dashed line, simplified Kubo-Greenwood formula, Eq. (2.15), which predicts a second-order pole $\sigma(\omega)\propto 1/\omega^2$. Dotted line, results from Ref. [10], which used an interpolating procedure to extend the results of the Kubo-Greenwood approach to the static approximation described by the Ziman formula, Eq. (3.1). Dot-dashed line, prediction of Eq. (4.8).

III. CONDUCTIVITY AT ULTRALOW FREQUENCIES

A. Ziman formula

Consider the static limit $\omega=0$. The Ziman formula, which describes the conductivity due to electron-atom scattering, reads

$$\sigma(0) = \frac{2e^2}{3}\int v^2 \tau_p\left(-\frac{\partial f}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}. \tag{3.1}$$

One observes its drastic distinctions from the result of the Kubo-Greenwood-type approach. First, the Ziman formula, Eq. (3.1), gives a constant static limit for the conductivity, while the Kubo-Greenwood formula, Eq. (2.15), diverges at $\omega=0$. Second, in these two formulas the conductivity shows an opposite dependence on the relaxation time; Eq. (2.15) reveals an inverse dependence, $\propto 1/\tau_p$, while the Ziman formula (3.1) predicts a linear dependence, $\propto \tau_p$.

To find an origin for these distinctions, let us note that deriving Eq. (2.15) we assumed that the electron momentum $\boldsymbol{p}$ is a good quantum number, which is changed only due to scattering on one given atom. Generally speaking, this assumption is incorrect. The momentum can be changed due to scattering on other atoms as well.

To see the implications of this fact more clearly, let us note that the second-order pole $\propto 1/\omega^2$ in the conductivity arises as a direct consequence of the first-order pole $\propto 1/\omega$ in the amplitude. The latter can be written as an integral

$$\frac{1}{\omega} = -i\int_{-\infty}^{0} \exp(-i\omega t)dt, \tag{3.2}$$

where $|t|$ gives a period of time, which precedes an electron collision with the given atom. Equation (3.2) shows that de-

riving Eq. (2.15) one presumes that during all this period of time, which can be very large, up to infinity, the electron momentum remains constant.

As a matter of fact, this is not true. The momentum can remain constant only over a finite period of time, which equals a typical interval of time between two subsequent collisions. This interval is measured by the relaxation time. This means that the relaxation time should necessarily produce the cutoff for the integral over time in Eq. (3.2):

$$-i\int_{-\infty}^{0}\exp(-i\omega t)dt \to -i\int_{-\tau_p}^{0}\exp(-i\omega t). \tag{3.3}$$

The cutoff procedure can be fulfilled slightly differently and more conveniently by introducing the cut off function in the integrand:

$$-i\int_{-\infty}^{0}\exp(-i\omega t)dt \to -i\int_{-\infty}^{0}\exp(-i\omega t-|t|/\tau_p)=\frac{1}{\omega+i/\tau_p}. \tag{3.4}$$

The pole at $\omega=0$, which exists on the left-hand side here, is replaced by a finite behavior of the right-hand side.

These simple arguments show that the pole $\propto 1/\omega$ in the scattering amplitude and, correspondingly, the second-order pole $\propto 1/\omega^2$ in the conductivity are closely related to the single-atom approximation. The many-atomic events lead to the relaxation time, which erases this pole behavior. This argument is developed below, in Sec. IV.

IV. RESONANT STATES OF CONDUCTING ELECTRONS

According to Sec. III A, multiple-scattering events should play an important role in the ultralow-frequency region. In order to account for this scattering, let us start from a simple physical picture. If the electron has the momentum $\boldsymbol{p}$, then it keeps this momentum only for some finite period of time (relaxation time) because collisions with atoms in a plasma inevitably change it. In the classical approximation this implies that only some finite part of the classical trajectory of the electron can be described by the initial momentum, while longer parts of the trajectory "forget" this momentum. Similarly, in a quantum description, the stationary quantum states describing electron propagation in a plasma cannot be characterized by the momentum.

However, if the plasma is sufficiently transparent—i.e., the relaxation time is sufficiently large—then during long intervals of time the electron momentum on classical trajectories remains constant. Consequently, the quantum states, which describe the electron propagation in a region outside atomic cores during moments of time separating consequent collisions, should look similar to conventional plane waves. The fact that collisions, which destroy the electron momentum, are essential can be accounted for by stating that a quantum state with the given momentum $\boldsymbol{p}$ exists only during a finite period of time. In other words, the electron wave function of the conducting electron outside the atomic core of some atom resembles a conventional plane wave, but with the restriction that it exist only during a finite period of time that equals the relaxation time. Presuming that the relaxation time is large, one can say that this wave function is a quasistationary state, which is similar to a plane wave, but possesses a finite width Γ_p defined by the relaxation time

$$\frac{\Gamma_p}{2}=\frac{\hbar}{\tau_p}. \tag{4.1}$$

This identity, combined with Eq. (2.14), states simply that $\Gamma_p=2\hbar v n_a \sigma_{tr}$, which makes sense.

The arguments just presented show that the electron wave function outside the atomic core of some atom can be written in a form

$$|\boldsymbol{p},t\rangle=\exp\left(i(\boldsymbol{p}\cdot\boldsymbol{r}-E_p t)-\frac{\Gamma_p}{2}t\right). \tag{4.2}$$

This simple wave function possesses important physical properties. First, it is close to a plane wave. Second, its finite width accounts for multiple-scattering events—i.e., collisions with different atoms. The width of this resonant state is described by the relaxation time, Eq. (4.1); the larger is the relaxation time, the closer is the wave function to a plane wave, exactly what one should expect when collisions are rare.

The above argument can be developed further. If one wishes to consider the electron wave function in a close vicinity of a given atom, then the plane wave should be replaced by the wave function which takes into account the influence of the atomic potential $U(\boldsymbol{r})$. In other words, one needs to make in Eq. (4.2) a substitution $\exp(i\boldsymbol{p}\cdot\boldsymbol{r})\to\psi_p(\boldsymbol{r})$. As a result, the wave function of a conducting electron, which takes into account the potential of a given atom, as well as scattering by other atomic particles, has the following form:

$$\Psi_p(\boldsymbol{r},t)=\psi_p(\boldsymbol{r})\exp\left(iE_p t-\frac{\Gamma_p}{2}t\right). \tag{4.3}$$

Let us repeat, $\psi_p(\boldsymbol{r})$ here is the wave function, which describes the electron behavior in the potential created by a single atom, while Γ_p is the width, which describes the momentum relaxation due to scattering processes on all atoms.

It is instructive to compare Eq. (4.3) with a simple, classical idea of relaxation of the momentum. Consider for this purpose a value of the momentum averaged over the wave function, Eq. (4.3):

$$\boldsymbol{P}(t)=\frac{1}{V}\int_V \Psi^*(\boldsymbol{r},t)\boldsymbol{p}\Psi(\boldsymbol{r},t)d^3r. \tag{4.4}$$

Here $\boldsymbol{p}$ is the operator of the electron momentum and V is a large, but finite volume, which makes the ratio in Eq. (4.4) well defined and V independent. From Eqs. (4.3) and (4.4) one immediately finds that $\boldsymbol{P}(t)=\exp(-\Gamma_p t/\hbar)\boldsymbol{P}(0)$. The above can be written in a more routine form

$$\frac{d\boldsymbol{P}(t)}{dt}=-\frac{1}{\tau_p}\boldsymbol{P}(t). \tag{4.5}$$

Clearly, this expresses a relaxation of the electron momentum in conventional classical terms; τ_p plays here a role of

the classical relaxation time, as one should have expected. Thus, a quantum description of the relaxation of the electron momentum based on the wave function, Eq. (4.3), reproduces a well-known conventional classical picture.

Using the wave function Eq. (4.3), in the Kubo-Greenwood formalism, one can follow a path outlined in Sec. II B. However, a well-known shortcut makes these calculations redundant. A quasistationary nature of the wave function, Eq. (4.3), indicates that an amplitude of any resonant process involving this state acquires a conventional resonant energy denominator:

$$\frac{1}{\Delta E + i\Gamma_p/2}. \tag{4.6}$$

Here ΔE is a deviation of energy from its resonant value, which is presumed to be low. In our case this deviation is defined by the frequency of the electromagnetic field $\Delta E = \hbar\omega$. The resonant factor, Eq. (4.6), coincides with the one found in Eq. (3.4), which underlines again a main physical idea: the multiple-scattering events allow the electron momentum to exist only during a finite period of time.

The resonant amplitude, Eq. (4.6), always brings into the probability the resonant factor

$$\frac{1}{\Delta E^2 + \Gamma_p^2/4}, \tag{4.7}$$

which is often called the Breit-Wigner factor (in atomic physics this describes Lorentzian lines).

Applying Eq. (4.7) to the process at hand, one takes Eq. (2.15) and, making the substitution $1/\omega^2 \to 1/(\omega^2+\Gamma_p^2/4)$, arrives at the following result:

$$\sigma(\omega) = \frac{2e^2}{3}\int \frac{v^2\tau_p}{\omega^2\tau_p^2+1}\left(-\frac{\partial \mathsf{f}}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}. \tag{4.8}$$

As mentioned earlier, the above result can be obtained directly using the wave function, Eq. (4.3), in the Kubo-Greenwood formalism; however, the abbreviated derivation based on Eq. (4.7) makes the discussion more transparent.

Equation (4.8) differs from Eq. (2.15), which was derived in the single-atom approximation, by the only physical fact; it accounts for many-atom collisions. This distinction becomes crucial in the static limit, allowing Eq. (4.8) to reproduce correctly the Ziman formula, Eq. (3.1). Thus, we return to the statement, which was mentioned several times previously: the many-atom events are very important for low frequencies. In contrast, in the high-frequency region $\omega\tau_p > 1$, Eq. (4.8) reproduces Eq. (2.15), which is based on the simple single-atom approximation. Thus, for $\omega\tau_p > 1$ the many-atom events become irrelevant, in agreement with discussion in Secs. I and II B.

The arguments above could have been developed in a less verbose fashion by starting from average-atom picture in a suitably chosen optical potential; however, the present approach has the advantage of modifying the unsatisfactory parts of the existing model while leaving the satisfactory parts (those related to bound-bound and bound-free contributions to the conductivity) intact.

Optical properties of a plasma are conveniently described with the help of a complex conductivity, which allows one to define the complex refraction index. Using Eq. (4.8) for the real part of the conductivity and applying the conventional Kramers-Kronig dispersion relation [28–32], one finds that its real and imaginary parts may be written side by side:

$$\begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix}\sigma(\omega) = \frac{2e^2}{3}\int \begin{Bmatrix} \mathrm{Re} \\ \mathrm{Im} \end{Bmatrix}\frac{iv^2\tau_p}{\omega\tau_p + i}\left(-\frac{\partial \mathsf{f}}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}. \tag{4.9}$$

Equation (4.8) is one of the main results of this work. Its simple nature inspires a feeling that it could have been written without any discussion, as a simple convenient interpolation between the Ziman formula, Eq. (3.1), and the results of the Kubo-Greenwood approach, Eq. (2.15). However, it is rewarding to realize that this result follows from a clear physical idea, which states that a conducting electron can possess a constant momentum only over a finite period of time.

Several remarks should be made concerning our result for the low-frequency conductivity. First, it should be noted that the classical Drude model leads to the expression

$$\sigma_{\mathrm{Drude}}(\omega) = \frac{e^2}{m}\frac{\tau}{\omega^2\tau^2+1}$$

for the frequency-dependent conductivity per electron, where τ is a classical relaxation time. Thus, Eq. (4.8) can be viewed as a thermal average of the Drude conductivity. Second, it was shown by Smith [33], where multiple-scattering events were described by a Poisson distribution, that the classical Drude conductivity maximum can, under certain conditions, move away from $\omega=0$. A similar shift of the conductivity maximum is found in molecular dynamics simulations and in certain experiments. The fact that the low-frequency conductivity predicted by Eq. (4.8) always takes on its maximun value at $\omega=0$ represents a shortcoming of the formalism.

V. SUM RULE

Using Eq. (4.8), one can calculate a simple but important integral

$$\int_0^\infty \sigma(\omega)d\omega = \frac{\pi}{3}e^2\int v^2\left(-\frac{\partial \mathsf{f}}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}. \tag{5.1}$$

Rewriting here $d^3p = m^2 v dE_p d\Omega$ and integrating over the energy by parts, one finds

$$\begin{aligned}\int_0^\infty \sigma(\omega)d\omega &= \frac{\pi}{3}e^2m^2\int v^3\left(-\frac{\partial \mathsf{f}}{\partial E}\right)\frac{d\varepsilon d\Omega}{(2\pi\hbar)^3} \\ &= \frac{\pi}{3}\frac{e^2}{m}\int p^3\left(-\frac{\partial \mathsf{f}}{\partial E}\right)\frac{d\varepsilon d\Omega}{(2\pi\hbar)^3} \\ &= \pi e^2\int p\mathsf{f}\frac{d\varepsilon d\Omega}{(2\pi\hbar)^3} = \frac{\pi e^2}{m}\int \mathsf{f}\frac{d^3p}{(2\pi\hbar)^3}.\end{aligned} \tag{5.2}$$

Taking into account Eq. (2.12), one finds that Eq. (5.2) represents the known, conventional conductivity sum rule

$$\frac{2}{\pi}\int_0^\infty \sigma(\omega)d\omega = \frac{n_c e^2}{m}. \tag{5.3}$$

The integration in Eq. (5.3) includes the region of very high frequencies, above the limit in Eq. (1.1), which cannot be reliably covered by Eq. (4.8). However, this region gives only a small contribution to the sum rule because at high frequencies the integration in Eq. (5.3) converges very well, as $\int d\omega/\omega^2$. The sum rule, Eq. (5.3), supports the validity of Eq. (4.8).

VI. SUMMARY

Let us summarize the main physical ideas. In the vicinity of a given atom the wave function of a conducting electron is strongly influenced by the potential of this atom. This fact makes it natural to presume that the problem can be formulated with the help of an average-atom model, which accounts for this variation and describes correctly the electron scattering on this atom. However, the conductivity is related to processes of absorption and emission of electric field quanta during scattering of the conducting electron by a given atom. When the frequency of the field is ultralow, the absorption and emission take place in a region located far away from the atom. The electron wave function in this region is necessarily influenced by potentials of other atoms. As a result, the lower the frequency is, the more important are the many-atom events. Thus, the *naive* single-atom approximation inevitably breaks down in the static limit, where multiple scattering becomes crucial.

From the first glance, the necessity to account for multiple scattering should make things much more complicated for the theory. There is though an important simplification. The many-atom events manifest themselves mainly via a restriction, which they put on the period of time during which the conducting electron can possess a given momentum. Henceforth, one can account for these events by stating that the wave function of a conducting electron is a quasistationary state, which exists only during a large, but finite period of time, which equals the relaxation time for the momentum. This idea can be expressed in terms of the quasistationary state, Eq. (4.3), which describes the conducting electron. As a result, it becomes possible to account for multiple scattering within the formalism of the average-atom approximation, which greatly simplifies the problem.

Applying this idea within the framework of the Kubo-Greenwood formalism, we find that the conductivity is given by Eq. (4.8), which possesses several interesting properties.

(i) In the static limit it reproduces the Ziman formula, Eq. (3.1).

(ii) In the high-frequency region it is reduced to the Kubo-Greenwood-type formula, Eq. (2.15), derived within the *naive* average-atom approximation.

(iii) It satisfies the conventional sum rule, Eq. (5.3).

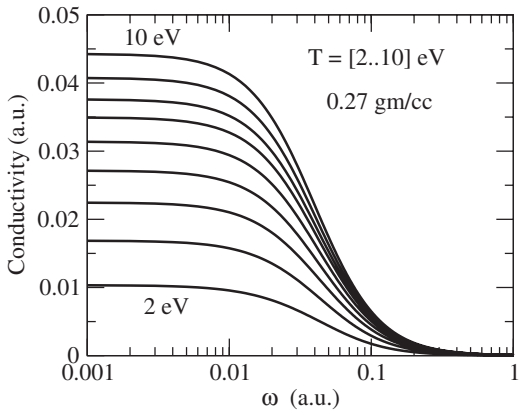

FIG. 3. The conductivity of an aluminum plasma at different temperatures. Calculations are based on Eq. (4.8). The parameters used in this formula are evaluated with the help of the approach of Ref. [10].

(iv) It is formulated in terms of physical quantities, which can be evaluated in the average-atom approximation that is convenient for applications.

Our starting point was Eq. (2.4), which relates the elastic-scattering amplitude with the amplitude of absorption (emission) of low-frequency quanta. The latter gives a particular example of a general property of QED, which allows one to express any radiation process with soft quanta via a purely elastic scattering process; see, e.g., [27]. Starting from Eq. (2.4), we derive Eq. (2.15) using a single-atom approximation, then taking into account many-atom events upgrade it to Eq. (4.8), which, in the static limit, reproduces the Ziman formula, Eq. (3.1), for Ohm's law. Thus, the well-known, conventional Ohm's law may be considered as a direct consequence of general, fundamental infrared properties of QED.

Using Eq. (4.8) and evaluating the necessary average-atom quantities τ_p and f_p with the help of the model of Ref. [10] we calculated the conductivity of the aluminum plasma at different temperatures. The results are shown in Figs. 2 and 3. In the one-atom approximation the conductivity is divergent as $\sigma \propto 1/\omega^2$, as shown in the solid and dashed lines in Fig. 2. To avoid this unphysical divergence Ref. [10] suggested a particular interpolating procedure, shown by a dotted line in Fig. 2, which brings the conductivity to the Ziman formula, Eq. (3.1), in the static limit. Equation (4.8) provides a more rigorous treatment of the conductivity at low frequencies, which does not rely on an interpolation. It is satisfying that the two approaches give close numerical results; compare the dotted and dot-dashed lines in Fig. 2.

Figure 3 presents results of a series of calculations based on Eq. (4.8) for different temperatures of the plasma. The increase of the conductivity with temperature reflects an increase of the concentration of conducting electrons. The rapid decrease of the conductivity in the high-frequency region underlines the important role played by low frequencies; as was mentioned, the low-frequency region gives a dominant contribution to the sum rule, Eq. (5.3).

In conclusion, it is shown that Eq. (4.8) successfully describes plasma conductivity at low frequencies.

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