Analytical expression for high-frequency dielectric function of metals at moderate temperatures

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Abstract. Analytical expressions are derived for the dielectric function of metals at moderate temperatures, determined by electron–phonon interactions, taking a quantum statistical approach and linear response theory as a basis. The obtained formulas permit one to calculate an effective electron–phonon collision frequency and the dielectric function of two-temperature plasmas for arbitrary laser radiation frequencies. Different limiting cases are considered.

1. Introduction

Knowledge on the dielectric function (DF) of matter in wide ranges of frequencies, temperatures and densities is necessary for the description of experiments, where material is radiated with energetic charged particles or high power laser beams, which have been planned and discussed widely during past years, see, e.g., [1–6]. Extensive space and time-scale simulations are effectively conducted by means of hydrodynamic codes, which require relatively simple models of the DF to be used with them. An attempt to construct such a model, applicable within a wide-temperature range, was conducted in [7], but the DF approximations proposed were semi-empirical ones. The construction of a wide-range model for the DF based on first principles is still an open question.

Within a previous work [8], a successive (based on first-principles) derivation of model for the DF, which is valid for a wide range of frequencies (from infrared to ultraviolet), was presented. The model is sufficiently simple for use in hydrodynamic codes. It gives expressions for both the real and imaginary parts of the complex effective collision frequency and it fulfils Kramers–Kronig relations and sum rules.

On the other hand, the model [8], which is based on a Hamiltonian with electron–electron and electron–ion interaction, is of limited applicability at $T_e < E_F$ (where $T$ and $E_F$ are temperature of electrons and Fermi energy, respectively) because it does not take into account electron–phonon interactions. Particularly, this model overestimates the real part of the complex Drude-
like effective collision frequency \( \nu_{\text{Dr}} = \nu_{\text{Dr}}^0 + i \nu_{\text{Dr}}' \) with

\[
\nu_{\text{Dr}}^0(\omega) = \omega \Im \left\{ \frac{(n/n_c)(1 - \varepsilon(\omega))^{-1}}{\omega + i \nu(\omega)} \right\},
\nu_{\text{Dr}}'(\omega) = \omega \Re \left\{ 1 - \frac{(n/n_c)(1 - \varepsilon(\omega))^{-1}}{\omega + i \nu(\omega)} \right\},
\]

where \( n \) and \( n_c = m \omega^2/(4 \pi e^2) \) are concentrations of electrons and critical concentration, respectively, \( e \) and \( m \) are charge and mass of electrons, respectively, \( \omega \) is the laser frequency, \( \varepsilon \) is the DF. This approximation overestimates the absorption coefficient at low temperatures, see [8] for more details. Therefore elaboration of DF model on the base of the same quantum statistical approach and linear response theory, but with account for electron–phonon interactions is of high importance.

The approach used in this paper utilises the same linear response theory and quantum statistical operator method, as in the previous paper [8], devoted to DF for higher temperatures. Unlike classical kinetic approaches [9], this method provides a consistent description for the real and the imaginary part of the effective complex electron–ion collision frequency, see [8] for details. As it was recently demonstrated in [10], with respective to the choice of observables, this method can give rise to equations having the form of quantum kinetic equations, and in this sense it is in analogy to the method of quantum kinetic equation used e.g., in [11].

### 2. Basic equations

In the long-wavelength limit (i.e., neglecting spatial dispersion, the wave vector of the perturbation \( k \to 0 \)) quantum-statistical approach and the linear response theory gives an expression for the DF in the form of the generalized Drude formula [8, 12, 13]

\[
\lim_{k \to 0} \varepsilon(k, \omega) = \varepsilon(\omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega^2 + i \nu(\omega)},
\]

where \( \omega_{\text{pl}} = \sqrt{4 \pi n e^2 / m} \). The complex effective collision frequency \( \nu(\omega) \) is expressed through the dimensionless correlation functions \( \mathfrak{M}_{nm} \) and \( \mathfrak{C}_{nm} \) and dimensionless response parameters \( F_m \):

\[
\nu(\omega) = \nu_1(\omega) r_{\omega}(\omega),
\nu_1(\omega) = \omega_{\text{au}} \frac{\mathfrak{C}_{11}}{\mathfrak{M}_{11}},
\]

\[
r_{\omega}(\omega) = \frac{\mathfrak{M}_{11} 1 + i \omega^* \sum_m \mathfrak{M}_{1m} F_m}{\sum_m \mathfrak{M}_{1m} F_m},
\]

where \( \mathfrak{M}_{nm} = \left( \frac{\hat{P}_n; \hat{P}_m}{mnT} \right) \), \( \mathfrak{C}_{nm}(\omega) = \left( \frac{\hat{P}_n; \hat{P}_m}_{\omega+i\eta} \right) e^{i\eta \omega_{\text{au}}}, \) \( F_m = \frac{mT}{eE} F_m \), and \( F_m \) is response parameter, \( \omega_{\text{au}} \) is the atomic unit of frequency, \( \eta \) is an infinitesimal small positive value, \( h \omega_{\text{au}} = E_H = me^4/h^2 \approx 27.2 \text{ eV} \) is Hartree energy, \( h \) is the Planck constant, \( \omega^* = \omega / \omega_{\text{au}} \) is dimensionless frequency and \( E \) is electric field intensity. \( \hat{P}_n \) is the n-th momentum operator in the long-wavelength approximation:

\[
\hat{P}_n = \sum_p \hbar p (\beta E_p)^{(n-1)/2} \hat{n}_p,
\]

where \( \beta = 1/T \); \( E_p = \hbar p^2/(2m) \). \( \hat{n}_p = \hat{a}_p^+ \hat{a}_p, \hat{a}_p^+ \) and \( \hat{a}_p \) are creation and annihilation operators of electrons with the wave vector \( p \). Correlation functions of operators \( \hat{A}, \hat{B} \) are defined as a Kubo scalar product,

\[
(\hat{A}(t); \hat{B}) = \int_0^1 \left[ \text{Tr} \left\{ \hat{A}(t - i\hbar \tau) \hat{B} \hat{\rho}_0 \right\} \right] d\tau,
\]

(6)
and its Laplace transform,
\[
\langle \hat{A}; \hat{B} \rangle_z = \int_0^\infty dt e^{zt} \left( \hat{A}(t) \hat{B} \right),
\]
where \( \hat{A}(t) = e^{i\hat{H}t/\hbar} \hat{A} e^{-i\hat{H}t} \) is Heisenberg representation of the operator, \( \hat{\rho}_0 \) is equilibrium statistical operator,
\[
\hat{\rho}_0 = Z^{-1} \exp[-(\hat{H} - \mu \hat{n})/T], \quad Z = \text{Tr}\{e^{-(\hat{H} - \mu \hat{n})/T}\},
\]
\( Z \) is partition function; \( \hat{n} = \sum_p \hat{n}_p, \mu \) is chemical potential, and \( \hat{H} \) is Hamiltonian.

Response parameters are determined from the solution of the infinite system of equations [8, 10, 12–14]:
\[
\sum_m \left[ \mathcal{C}_{nm} - i\omega^* \mathcal{M}_{nm} \right] \mathcal{F}_m = \mathcal{M}_{n1}.
\]

The complex effective collision frequency of electrons \( \nu_1 \), see equation (2), is determined by the first moment (\( n = 1 \) in (5)) of the single-particle density matrix \( \hat{n}_p \). The correction factor \( r_\omega \) determines the contribution of higher moments. Earlier it has been shown [10, 13], that the inclusion of only 2 moments, \( \mathbf{P}_1 \) and \( \mathbf{P}_3 \), is sufficient for an accuracy of less than several %. In this case, from the above equations, it follows that
\[
r_\omega(\omega) = \frac{1}{\mathcal{C}_{11}} + \frac{i\omega Q_\omega}{Q_\omega},
\]
\[
Q_\omega = \frac{\mathcal{A}_{33} - 2\mathcal{A}_{31}\mathcal{A}_{31} + \mathcal{M}_{31}^2\mathcal{A}_{11}}{\mathcal{A}_{11}\mathcal{A}_{33} - \mathcal{M}_{31}^2},
\]
\[
\mathcal{M}_{lm} = \mathcal{C}_{lm} - i\omega^* \mathcal{M}_{lm}, \quad l, m \geq 1.
\]

The correlation functions \( \mathcal{M}_{lm} \) can be expressed as [14]
\[
\mathcal{M}_{lm} = \frac{\Gamma[(l + m + 3)/2]}{\Gamma(5/2)} \frac{I_{(l+m-1)/2}(\epsilon_\mu)}{I_{1/2}(\epsilon_\mu)}, \quad l, m \geq 1,
\]
\[
\mathcal{M}_{11} = 1, \quad \mathcal{M}_{31} = 5 I_{3/2}(\epsilon_\mu) / 2 I_{1/2}(\epsilon_\mu), \quad \mathcal{M}_{33} = 35 I_{5/2}(\epsilon_\mu) / 4 I_{1/2}(\epsilon_\mu),
\]
where \( \epsilon_\mu = \mu/T; I_\nu(y) = \Gamma(\nu+1) \int_0^\infty x^\nu [e^{x-y}+1]^{-1} dx \) are Fermi integrals; dimensionless chemical potential is expressed through the reverse function \( X_{1/2}(x) \) of the Fermi integral \( I_{1/2}(x) \),
\[
\epsilon_\mu = X_{1/2} \left( 2\epsilon_F^{3/2} / 3 \right),
\]
where \( \epsilon_F = E_F/T, \epsilon_F = \hbar^2(3\pi^2n)^{2/3}/(2m) \). In the non-degenerate case \( I_\nu(\epsilon_\mu) = e^{\epsilon_\nu} \), \( \mathcal{M}_{31} = 5/2, \mathcal{M}_{33} = 35/4, \) see [10].

To calculate the correlation functions due to electron–phonon interactions, the well-known Fröhlich Hamiltonian [15] was used:
\[
\hat{H} = \sum_{k,i} E_{k,i} \hat{a}_{k,i}^+ \hat{a}_{k,i} + \sum_{k,q,\lambda} \hbar \omega_q,\lambda \hat{b}_{q,\lambda}^+ \hat{b}_{q,\lambda} + \sum_{k,q,i,i',\lambda} g_{k}(q,i,i',\lambda) \hat{a}_{k,q,i}^+ \hat{a}_{k,i',\lambda}(\hat{b}_{q,\lambda}^+ + \hat{b}_{q,\lambda}),
\]
where \( k, q \) are wave vectors, \( i, i' \) are zone numbers, \( \lambda \) is the phonon mode number, \( \hat{a}_{k,i}^+, \hat{a}_{k,i} \) and \( \hat{b}_{q,\lambda}^+, \hat{b}_{q,\lambda} \) are creation and annihilation operators of electrons and phonons, respectively, \( E_{k,i} \) and \( \omega_{q,\lambda} \) are energy of electrons in \( i \)-th zone and frequency of phonon of \( \lambda \)-th mode, respectively,
\[
E_{k,i} = \hbar^2 k^2 / (2m \Xi_i) + E_{0,i},
\]
\( \Xi_i \)
m_i is the ratio of the electrons effective mass in the i-th zone to the free electron mass. \( E_{0,i} \) is the energy of the bottom of the i-th zone (for conductivity zone it can be assumed to be zero) and \( g_k(q,i,i',\lambda) \) is the coefficient of the electron–phonon interaction.

Performing the respective calculations in first Born approximation, the correlation function is expressed in terms of the occupation numbers of electrons and phonons. As a result, a general expression for the dimensionless correlation function, containing, generally speaking, the sum over different electronic zones and phonon modes is obtained, see Appendix A for details, as

\[
C_{NM} = \frac{2i}{\hbar^2 \omega_{au}} \sum_{p,q} \frac{N-1}{p+q} \left( p_z + q_z \right) \varepsilon_{\frac{p+q}{p+q}} \left( p_z - q_z \right) \sum_{i,n,\lambda} g_p(q, n, i, \lambda) g_{p+q}(q, i, n, \lambda)
\]

\[
\times \left\{ \frac{n_{p+q,n}(1 - n_{p,i}) + (n_{p+q,n} - n_{p,i})N_{q,\lambda}}{(p + q)^2/m_n - p^2/m_i + 2m(\omega_n,i - \alpha \omega_{q,\lambda})/\hbar} \left[ \frac{1}{\omega - \Delta_{p,i,-}^{p+q,n} + i\eta} + \frac{1}{\omega + \Delta_{p,i,-}^{p+q,n} + i\eta} \right] \right\}, \quad \text{(15)}
\]

where \( \varepsilon_p \equiv E_p/T, \) and below \( \varepsilon_{p,n} \equiv E_{p,n}/T, \varepsilon_{0,n} \equiv E_{0,n}/T; \]

\[
\Delta_{p,i,\pm}^{p+q,n} = \frac{\hbar}{2m} \left( (p + q)^2/m_n - p^2/m_i \right) + \omega_n,i \pm \omega_{q,\lambda}, \quad \omega_n,i = \frac{2m}{\hbar^2}(E_{0,n} - E_{0,i}),
\]

\( T_{ion} \) is the temperature of ions, \( \alpha = T/T_{ion}, n_{p,n} \) and \( N_{q,\lambda} \) are occupation numbers of electrons and phonons, respectively,

\[
n_{p,n} = \left[ 1 + e^{\varepsilon_{p,n} - \varepsilon_{p,n}} \right]^{-1}, \quad N_{q,\lambda} = \left[ e^{\omega_{q,\lambda}/T} - 1 \right]^{-1}, \quad \text{(16)}
\]

where \( E_{p,n} \) is given by (14).

In the case of transitions with a single phonon mode containing longitudinal optical phonons with a frequency independent of the wave vector [15], the correlation function is considered in the single-moment approximation, \( N = M = 1 \) in (15). Besides that, we disregard \textit{interband} transitions between different zones \( n,i \) and consider only the contribution due to free-free transitions in the conductivity zone. Furthermore, we assume the effective mass of different zones to be equal, \( m_n = m_i = m_\ast \). In this case, a fairly simple formula for \( C_{11} \) is obtained, which is similar to the analogous result for the screened Born approximation with a Hamiltonian containing electron–electron and electron–ion interactions, see [8]. We find

\[
C_{11} = \frac{\varepsilon_{inf}^{3/2}}{2\pi^{3/2}} \omega_{au} \varepsilon_{\infty,0,0} \int_0^\infty \int_0^\infty \frac{1}{w - x + w_{LO} + i\eta} + \frac{1}{w + x - w_{LO} + i\eta} \frac{(e^{4x} - 1)^{-1} - (e^{4\omega_{LO}} - 1)^{-1}}{x - \alpha w_{LO}} \ln \left[ 1 + \exp[\varepsilon_{\mu} - (y - x/y)^2] \right] \frac{1 + \exp[\varepsilon_{\mu} - (y - x/y)^2]}{1 + \exp[\varepsilon_{\mu} - (y + x/y)^2]} dxdy,
\]

where \( m_\ast \) is effective mass of electrons in the considered zone, \( \varepsilon_{inf,0} = \varepsilon_{inf}^{-1} - \varepsilon_0^{-1}, \varepsilon_{\infty} \) and \( \varepsilon_0 \) are dielectric constant at low frequencies due to interband transitions and full dielectric constant at low frequencies, respectively, \( w = \hbar \omega/(4T), \omega_{au} = \hbar \omega_{au}/T, w_{LO} = \hbar \omega_{LO}/(4T), \omega_{LO} \) is the frequency of longitudinal optical phonons.

In equation (17), the integral over \( dx \) can be performed applying the Sokhotskii–Plemey formula

\[
\int_{-\infty}^\infty \frac{f(x)}{x + i\eta} \ln(1 + \exp(\varepsilon_{\mu} - (y - x/y)^2)) dxdy = -i\pi f(0) + v.p. \int_{-\infty}^\infty \frac{f(x)}{x} dxdy
\]
to the first factor (where $vp$ denotes the principal value of the integral). In this case, real and imaginary part of the correlation function can easily be derived.

Note that the correlation functions dependencies on the temperature of electrons and the temperature of ions are determined, in accordance with their definitions, by the quantities $\lambda, w, w_{LO}, \tilde{w}_{au}, \alpha$. Unlike in a usual phenomenological treatment, these dependencies are not reduced to simple proportionalties in the general case.

3. Real part of $C_{11}$ and its asymptotics

From above consideration, the real part of the correlation function is found to be

$$C_{11}' = \frac{\varepsilon^{-3/2}_{F} m_{e}^{2} \varepsilon_{\infty,0} w_{LO}}{2\pi^{3/2}} \sum_{\sigma = \pm 1} \left( e^{i[w_{LO} + \sigma w]} - 1 \right)^{-1} \left( e^{i4w_{LO} \alpha} - 1 \right)^{-1}$$

$$\times \int_{0}^{\infty} y \, dy \ln \left[ \frac{1 + \exp \left\{ \varepsilon_{\mu} - \left[ y - \frac{w_{LO} + \sigma w}{y} \right]^{2} \right\}}{1 + \exp \left\{ \varepsilon_{\mu} - \left[ y + \frac{w_{LO} + \sigma w}{y} \right]^{2} \right\}} \right]. \quad (18)$$

Below, different asymptotics of this formula are considered.

3.1. The case of small frequencies, $w \ll w_{LO}$, $w \ll 1$

Under these conditions one can disregard dependence on $w$. Resulting formula has different forms for $\alpha = 1$ and $\alpha > 1$:

$$C_{11}'(\alpha > 1) = \frac{\varepsilon^{-3/2}_{F} m_{e}^{2} \varepsilon_{\infty,0} w_{LO}}{2\pi^{3/2}} \sum_{\sigma = \pm 1} \left( e^{i[w_{LO} + \sigma w]} - 1 \right)^{-1} \left( e^{i4w_{LO} \alpha} - 1 \right)^{-1}$$

$$\times \int_{0}^{\infty} y \, dy \ln \left[ \frac{1 + \exp \left\{ \varepsilon_{\mu} - \left[ y - \frac{w_{LO} + \sigma w}{y} \right]^{2} \right\}}{1 + \exp \left\{ \varepsilon_{\mu} - \left[ y + \frac{w_{LO} + \sigma w}{y} \right]^{2} \right\}} \right], \quad (19)$$

$$C_{11}'(\alpha = 1) = \frac{\varepsilon^{-3/2}_{F} m_{e}^{2} \varepsilon_{\infty,0}}{2\pi^{3/2}} \sum_{\sigma = \pm 1} \left( e^{i[w_{LO} + \sigma w]} - 1 \right)^{-1} \left( e^{i4w_{LO} \alpha} - 1 \right)^{-1}$$

$$\times \int_{0}^{\infty} y \, dy \ln \left[ \frac{1 + \exp \left\{ \varepsilon_{\mu} - \left[ y - \frac{w_{LO} + \sigma w}{y} \right]^{2} \right\}}{1 + \exp \left\{ \varepsilon_{\mu} - \left[ y + \frac{w_{LO} + \sigma w}{y} \right]^{2} \right\}} \right]. \quad (20)$$

For $w_{LO} \ll 1$ and for $w_{LO} \gg 1$ formulas (19) and (20) give the following asymptotics:

$$C_{11}'(w_{LO} \ll 1) = \frac{\varepsilon^{-3/2}_{F} m_{e}^{2} \varepsilon_{\infty,0} w_{LO}}{2\pi^{3/2}} \ln(1 + e^{\varepsilon\mu}) \times \begin{cases} 1 & \text{at } \alpha = 1, \\ 1/\alpha & \text{at } \alpha > 1, \end{cases} \quad (21)$$

$$C_{11}'(w_{LO} \gg 1) = \frac{\varepsilon^{-3/2}_{F} m_{e}^{2} \varepsilon_{\infty,0} w_{LO}}{2\pi^{3/2}} \sum_{\sigma = \pm 1} \frac{1}{e^{i4w_{LO} \alpha} - 1} \times \begin{cases} 4w_{LO}, & \alpha = 1 \\ 1/(\alpha - 1), & \alpha > 1. \end{cases} \quad (22)$$

In all the above limiting cases, $C_{11}'$ is independent of $w$, i.e. the laser frequency.
3.2. The case of frequency equal to phonon frequency, \( w = w_{LO} \)
This case should be analysed separately because of the removable singularity in the denominator of Fermi function in (18) at \( \sigma = -1 \). In this case (18) leads to
\[
\mathcal{C}'_{11} = \frac{\varepsilon_F^{-3/2}}{\pi^{3/2}} \frac{m^2_{s}\varepsilon_{\infty,0}}{\omega_{s,0}^{-1/2}} \left\{ \frac{2}{\alpha} \ln \left( 1 + e^{\varepsilon_{\mu}} \right) \right. \\
\left. + \frac{(e^{4w_{LO}} - 1)^{-1} - (e^{4w_{LO}a} - 1)^{-1}}{\alpha - 2} \int_{0}^{\infty} y dy \ln \left[ \frac{1 + \exp \left( \varepsilon_{\mu} - [y - 2w_{LO}/y]^2 \right)}{1 + \exp \left( \varepsilon_{\mu} - [y + 2w_{LO}/y]^2 \right)} \right] \right\}. \tag{23}
\]
From (23) one has similar limits for large and low phonon frequencies:
\[
\mathcal{C}'_{11} = \frac{\varepsilon_F^{-3/2}}{\pi^{3/2}} \frac{m^2_{s}\varepsilon_{\infty,0}}{\omega_{s,0}^{-1/2}} \frac{1}{\alpha} \ln \left( 1 + e^{\varepsilon_{\mu}} \right) \times \left\{ \begin{array}{ll}
1, & w_{LO} \gg 1, \\
9/8, & w_{LO} \ll 1.
\end{array} \right. \tag{24}
\]
Note, that expression (24) is very similar to equation (21). Also one can note, that for the limits of low and high temperatures equation (24) can be rewritten as
\[
\mathcal{C}'_{11} \approx \frac{m^2_{s}\varepsilon_{\infty,0}}{\omega_{s,0}^{-1/2}} \frac{1}{\alpha} \times \left\{ \begin{array}{ll}
4/(3\pi^2), & T \gg E_{F}, \\
1/(\pi^{3/2} \varepsilon_{F}^{-1/2}), & T \ll E_{F}.
\end{array} \right. \tag{25}
\]

3.3. The case of large frequency, \( w \gg w_{LO}, w \gg 1 \)
One has for this case from (18):
\[
\mathcal{C}'_{11} = \frac{\varepsilon_F^{-3/2}}{\pi^{3/2}} \frac{m^2_{s}\varepsilon_{\infty,0}}{\omega_{s,0}^{-1/2}} \frac{1}{w_{LO}w^{1/2}} \\
\times \left[ 1 + \frac{(e^{4w_{LO}a} - 1)^{-1}}{w + w_{LO}a} + \frac{(e^{4w_{LO}a} - 1)^{-1} - (e^{4(w+w_{LO})} - 1)^{-1}}{w + w_{LO} - w_{LO}a} \right] \int_{0}^{\infty} dt \ln \left[ 1 + e^{\varepsilon_{\mu} - t^{2}} \right]. \tag{26}
\]
It is interesting to note, that in both limits of high and low temperatures equation (26) gives the same asymptotics:
\[
\mathcal{C}'_{11}(\varepsilon_F \ll 1 \text{ or } \varepsilon_F \gg 1) = \frac{1}{\pi^{3/2}} \left\{ \begin{array}{ll}
1/3, & w_{LO} \ll 1, \\
1, & \alpha w_{LO} \ll 1.
\end{array} \right. \tag{27}
\]

3.4. The case of small phonon frequencies, \( w_{LO} \ll 1, \alpha w_{LO} \ll 1 \)
This case is practically most important for laser–matter interaction, as long as for most cases phonon frequencies are less than room temperatures [16] (in energetic units).
In this case and for high laser frequencies (\( w \gg 1 \)) one has from (26):
\[
\mathcal{C}'_{11} = \frac{\varepsilon_F^{-3/2}}{4\pi^{3/2} \omega_{s,0}^{-1/2} w^{1/2} \alpha} \int_{0}^{\infty} dt \ln \left[ 1 + e^{\varepsilon_{\mu} - t^{2}} \right] \tag{28}
\]
\[
\approx \frac{1}{6} \frac{m^2_{s}\varepsilon_{\infty,0}}{\omega_{s,0}^{-1/2} w^{1/2} \alpha}. \tag{29}
\]
where the last expression follows from the one above by the same procedure, as (27) follows from (26).
Figure 1. Real part of the electron–phonon collision frequency (18) as a function of temperature of electrons for a solid-density \((\rho = 2.71 \text{ g/cm}^3)\) aluminum plasma with an average ion charge \(Z = 3\), ion temperature \(T_{\text{ion}} = 1 \text{ eV}\), for different laser photon energies \(\hbar \omega\) (shown on the legend). High-frequency (HF) asymptotics (29) for the same wavelength and low-frequency (LF) asymptotic (30) are shown by markers.

Expressions for small phonon frequencies and for low laser frequencies \((w \ll w_{\text{LO}}\) or \(w = w_{\text{LO}}\)) are already given above by (21) and (24). They can be rewritten as

\[
C_{11}^\prime = \frac{\varepsilon_{p}^{-3/2} m_{e}^{2} \varepsilon_{\infty, \text{0}}^{0}}{2\pi^{3/2}} \frac{1}{\varpi_{\text{a,a}}^{1/2}} \ln \left(1 + e^{\varepsilon_{\mu}}\right) \times \left\{ \begin{array}{ll} 1, & w \ll w_{\text{LO}}, \\ 9/4, & w = w_{\text{LO}}. \end{array} \right. \tag{30}
\]

Expressions (28)– (30) are proportional to ion temperature \(T_{\text{ion}}\). This proportionality holds in the general case, if besides inequalities \(w_{\text{LO}} \ll 1\) and \(\alpha w_{\text{LO}} \ll 1\) also the inequalities \(w \gg w_{\text{LO}}\) and \(w \gg \alpha w_{\text{LO}}\) are valid. In this case, from (18) one has:

\[
C_{11}^\prime = \frac{\varepsilon_{p}^{-3/2} m_{e}^{2} \varepsilon_{\infty, \text{0}}^{0}}{4\pi^{3/2}} \frac{1}{\varpi_{\text{a,a}}^{1/2}} \frac{1}{\alpha w} \ln \left[ \frac{1 + \exp \left( \varepsilon_{\mu} - \left( y - w/y \right)^{2} \right)}{1 + \exp \left( \varepsilon_{\mu} - \left( y + w/y \right)^{2} \right)} \right]. \tag{31}
\]

4. Numerical examples

As an example, the real part of the electron–phonon collision frequency is calculated within 1-moment approximation, \(\nu_{\text{e-ph}} = \nu_{1} = \omega_{\text{a0}} C_{11}\), by means of formula (18). The value of \(\varepsilon_{\infty}^{-3} - \varepsilon_{0}^{-3}\) is assumed to be 1, and the value of \(\omega_{\text{LO}}\) in aluminum was determined as the position of the maximum of the phonon spectrum for aluminum [16] and was equal \(\hbar \omega_{\text{LO}} \approx 0.006\) (remember that \(w_{\text{LO}} = \omega_{\text{LO}}/4\)). The result is shown in figure 1. The high-frequency asymptotics (29) for the same laser frequency and the low-frequency asymptotic (30) can also be seen.

Calculations were conducted for different temperatures of electrons, but with fixed temperature of ions \(T_{\text{ion}}\). In the considered case of small phonon frequencies, the value of \(\nu_{\text{e-ph}}\) is linearly increasing with increasing \(T_{\text{ion}}\), as it follows from (31). Real part of the effective electron–phonon collision frequency \(\nu_{\text{e-ph}}^\prime\) is independent on the temperature of electrons \(T\) for high laser frequencies (high-frequency case (29)), and is decreasing with increasing \(T\) for high temperature and low laser frequencies (at laser wavelength \(\lambda > 0.01 \mu\text{m}\)), see figure 1.
Phenomenological considerations [17–19] show, that with inclusion of Umklapp process the effective electron–phonon collision frequency should be increasing, rather than decreasing. The study of this phenomenon will be the subject of our further activities.

5. Conclusions
Simple expressions for the correlation functions and DF are obtained using quantum statistical approach, linear response theory and Fröhlich Hamiltonian for electron–phonon interactions in the 1-st Born approximation for the case of moderate and low temperatures, when electron–phonon interactions are important.

The results obtained can be incorporated within a consequent (from first principles) derivation of a wide-range model for the DF, covering both temperatures above and below the Fermi energy for a dense plasma, and simultaneously applicable in a wide frequency range, from infrared to ultraviolet radiation.

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Appendix
Derivation of expressions (15) and (17) for correlation functions.

The correlation functions $c_{nm}$ (4) can be expressed via commutators of Hamiltonian (13) with the density operators of electrons $\hat{n}_{p,i} = \hat{a}^+_p \hat{a}_{p,i}$ (where index $p$ stands for momentum and index $i$ stands for zone number):

$$c_{nm}(\omega) = \sum_{p,i,p',i'} \frac{p_z^i p_z^{i'} \varepsilon_{p,i}^{(n-1)/2} \varepsilon_{p',i'}^{(m-1)/2}}{mnT \omega \Omega_0} C_{(p,i,p',i')}$$

where $\varepsilon_{p,i} = \varepsilon_{p,i}/T = m_i^{-1} \hbar^2 p^2 / (2mT)$ is dimensionless energy of electrons at $i$-th zone and $\Omega_0$ is normalization volume.

The commutator of density operator with Hamiltonian (13) can be expressed as

$$[\hat{n}_{p,i}, \hat{H}] = \sum_{k,q,m,n,\lambda} g_k(q,m,n,\lambda) (\hat{b}^+_{q,\lambda} + \hat{b}^-_{q,\lambda}) (\delta_{k+q,p} \delta_{mn} - \delta_{k,p} \delta_{qn}) \hat{a}^+_{k,m} \hat{a}_{k+q,n}$$

where commutation relations for fermion creation and annihilation operators and their results in the form of

$$[\hat{n}_{p,m}, \hat{a}_{k,n}] = -\delta_{pk} \delta_{mn} \hat{a}_{p,n}, \quad [\hat{n}_{p,m}, \hat{a}^+_{k,n}] = \delta_{pk} \delta_{mn} \hat{a}^+_{k,n};$$

$$[\hat{n}_{p,m}, \hat{a}^+_{p_1,n_1} \hat{a}^-_{p_2,n_2}] = (\delta_{pp_1} \delta_{mn_1} - \delta_{pp_2} \delta_{mn_2}) \hat{a}^+_{p_1,n_1} \hat{a}^-_{p_2,n_2}$$

were used for derivation of (A.2). Similar expressions for commutation relations with phonon creation and annihilation operators are also used in the derivation:

$$[\hat{N}_{q,\lambda}, \hat{b}_{k,\lambda}] = -\delta_{qk} \delta_{\lambda\lambda'} \hat{b}_{k,\lambda'}, \quad [\hat{N}_{q,\lambda}, \hat{b}^+_{k,\lambda}] = \delta_{qk} \delta_{\lambda\lambda'} \hat{b}^+_{k,\lambda'},$$

where $\hat{N}_{q,\lambda} = \hat{b}^+_{q,\lambda} \hat{b}_{q,\lambda}$.

Besides that, Backer–Hausdorf theorem

$$e^{\hat{A}} \hat{C} e^{-\hat{A}} = \hat{C} + [\hat{A}, \hat{C}] + \frac{1}{2} [\hat{A}, [\hat{A}, \hat{C}]] + \frac{1}{3!} [\hat{A}, [\hat{A}, [\hat{A}, \hat{C}]]) + \cdots$$

for some operators $\hat{A}$ and $\hat{C}$ is also used in the subsequent derivation.
With (A.2) and (A.1) one has
\[
\mathcal{C}_{(p,i,p',i')} = \sum_{k,q,m,n,\lambda} g_k(q,m,n,\lambda) g_{k'}(q',m',n',\lambda') (\delta_{k+q,p} \delta_{m,n} - \delta_{k,p} \delta_{m',n'}) \times (\delta_{k'+q',p'} \delta_{m'+n'} - \delta_{k',p'} \delta_{m'+n'}) (\hat{b}_{q,\lambda}^+ + \hat{b}_{-q,\lambda}^+) \hat{a}_{k+q,m,\lambda} \hat{a}_{k,n,\lambda'} (\hat{b}_{q',\lambda'}^+ + \hat{b}_{-q',\lambda'}^+) \hat{a}_{k'+q',m',\lambda'} \hat{a}_{k',n',\lambda'} \omega + i\eta \quad (A.6)
\]

The correlation function in (A.6) is determined directly by definitions (6), (7), but in the considered 1-st Born approximation the equilibrium statistical operator \( \hat{\rho}_0 \) is used in the form
\[
\hat{\rho}_0 = \hat{\rho}_e \hat{\rho}_{ph}, \quad \hat{\rho}_e = Z_e^{-1} e^{-(\hat{H}_{0,e} - m \hat{n})}, \quad \hat{\rho}_{ph} = Z_{ph}^{-1} e^{-\hat{H}_{0,ph}}, \quad (A.7)
\]

where \( \hat{n}_{k,i} = \hat{a}_{k,i}^+ \hat{a}_{k,i}, \hat{n} = \sum \hat{n}_{k,i}, \hat{N}_{q,\lambda} = \hat{b}_{q,\lambda}^+ \hat{b}_{q,\lambda}^0 \), i.e., the electron–phonon interaction in (13) is accounted explicitly in expression (A.6) for \( \mathcal{C}_{(p,i,p',i')} \), but is omitted in expression for \( \hat{\rho} \).

From (A.3) and (A.4) one has the following expressions:
\[
\hat{H}_{0,e} = \sum_{k,i} \varepsilon_{k,i} \hat{n}_{k,i}, \quad \hat{H}_{0,ph} = \sum_{q,\lambda} \hbar \omega_{q,\lambda} \hat{N}_{q,\lambda} \quad (A.8)
\]

where condition \( \omega_{-q,\lambda} = \omega_{q,\lambda} \) is assumed for second equality.

Using (A.8), (A.5) and expressions (A.7), the correlation function of fermion and phonon creation and annihilation operators in expression (A.6) for \( \mathcal{C}_{(p,i,p',i')} \) can be rewritten as
\[
\langle \ldots \rangle_{\omega + i\eta} = n_{k+q,m}(1 - n_{k,n}) \delta_{q',-q} \delta_{k',k+q} \delta_{n',n} \delta_{\lambda',\lambda} (\hat{n}_{k+q,m} + (N_{q,\lambda} + 1) \hat{G}_{k,n}^{k+q,m}(\hat{b}_{q,\lambda}^+ - \hat{b}_{q,\lambda}^{-})) \quad (A.9)
\]

where
\[
\hat{G}_{k,n}^{k+q,m} = \frac{1 - n_{k+q,m}}{n_{k+q,m}} \frac{n_{k,n}}{1 + n_{k,n}} \left( \frac{1 + \tilde{N}_{q,\lambda}}{\varepsilon_{k+q,m} - \varepsilon_{k,n}} \right)^{1/2} \frac{i}{(\varepsilon_{k+q,m} - \varepsilon_{k,n})/T + \hbar \omega_{q,\lambda}/T_i + \Delta_{k,n,=}^{k+q,m} + i\eta}, \quad \Delta_{k,n,=}^{k+q,m} = \frac{\varepsilon_{k+q,m} - \varepsilon_{k,n}}{\hbar} \pm \omega_{q,\lambda} \quad (A.10)
\]

Substituting (A.9) into (A.6), one gets
\[
\mathcal{C}_{(p,i,p',i')} = -i \sum_{q,n,\lambda} g_p(q,n,i,\lambda) g_{p'}(q',n,i,\lambda) \left( \delta_{p',p} \delta_{q,n,i'} - \delta_{p',p} \delta_{q,n,i'} \right) \times \left\{ \frac{n_{p+q,n} - (1 - n_{p,i}) N_{q,\lambda}}{(\varepsilon_{p+q,n} - \varepsilon_{p,i})/T + \hbar \omega_{q,\lambda}/T_i + \Delta_{p,i,-}^{p+q,n} + i\eta} + \frac{1}{\omega - \Delta_{p,i,-}^{p+q,n} + i\eta} \right\} \left\{ \frac{n_{p+q,n} - (1 - n_{p,i}) N_{q,\lambda}}{(\varepsilon_{p+q,n} - \varepsilon_{p,i})/T + \hbar \omega_{q,\lambda}/T_i + \Delta_{p,i,-}^{p+q,n} + i\eta} + \frac{1}{\omega - \Delta_{p,i,-}^{p+q,n} + i\eta} \right\}, \quad (A.10)
\]

where equality \( g_p(q,n,i,\lambda) = g_p(-q,n,i,\lambda) \) (see [15]) was used in the derivation.

Substitution of (A.10) into (A.1) gives (15).

In order to derive expression (17) from (15), we consider single zone (disregard interband transitions) and single phonon mode (indexes \( i, n, \lambda \) are omitted). Also we make subsequent substitutions in different terms of (15):
\[
q \leftrightarrow -q, \quad p \leftrightarrow p + q, \quad p + q \leftrightarrow p, \quad p \leftrightarrow p + q; \quad \Delta_{p,-}^{p+q} \leftrightarrow -\Delta_{p,-}^{p+q}, \quad \Delta_{p,+}^{p+q} \leftrightarrow -\Delta_{p,+}^{p+q}; \quad p \leftrightarrow p - q/2
\]
and get the following expression for $C_{11}$:

$$C_{11} = \frac{-i/3}{\hbar^2 \omega_n n \Omega_0} \sum_q q^2 \sum_p g_{p-q/2}(q) g_{p+q/2}(q) \frac{n_{p+q/2}(1 - n_{p-q/2}) + (n_{p+q/2} - n_{p-q/2}) N_q}{\bar{p} q - \tilde{m} \omega q \alpha / \hbar} \times \left[ \omega - \hbar \tilde{p} q / m + \omega_q + \eta + \omega + \hbar \tilde{p} q / m - \omega_q + \eta \right].$$

(A.11)

In the next step we use cylindrical system of coordinate with axis $0\bar{z} || \bar{q}$ and replace sums over $p$ and $|q|$ in (A.11) by (we conserve designation $q$ for $|q|$ as long as it will not give rise to confusion in this case)

$$\sum_q \frac{\Omega_0}{(2\pi)^3} \int d^3q = \frac{\Omega_0}{2\pi^2} \int_0^\infty d^2q, \quad \sum_p = \frac{2\bar{\Omega}_0}{(2\pi)^3} \int d^3p = \frac{\bar{\Omega}_0}{2\pi^2} \int_0^\infty r dr \int_0^\infty ds,$$

(A.12)

where $r$ is the component of $\bar{p}$ perpendicular to $\bar{q}$ and $s$ is the component of $\bar{p}$ parallel to $\bar{q}$ (similar procedure of derivation was used in the work [10] for electron–ion and electron–electron correlation functions).

After substitution of (A.12) to (A.11) the integral over $s$ is done analytically and after some elementary mathematical transformations one gets (17), if one treat electron–phonon coupling functions $g_{p \pm q/2}(q)$ in (A.11) as independent of the component $r$ of $\bar{p}$ and use expression

$$g^2 = g_{LO}(q)^2 = \frac{2\pi e^2 \hbar \omega_{LO}}{q^2 \Omega_0} \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_0} \right)$$

(A.13)

for $g$ for the case of longitudinal optical phonons [15] and condition $\Omega_0 = n^{-1}$, where $n$ is the concentration of electrons.

References

[1] Krasyuk I K, Pashinin P P, Semenov A Yu, Khishchenko K V and Fortov V E 2016 Laser Phys. 26 094001
[2] Andreev N E et al 2015 Laser Part. Beams 33 541–50
[3] Ingomarov N A et al 2013 Contrib. Plasma Phys. 53 796–810
[4] Povarnitsyn M E and Andreev N E 2016 J. Phys.: Conf. Ser. 774 012105
[5] Andreev N E, Pugachev L P, Povarnitsyn M E and Levashov P R 2016 Laser Part. Beams 34 115–22
[6] Andreev N E, Povarnitsyn M E, Pugachev L P and Levashov P R 2015 J. Phys.: Conf. Ser. 653 012006
[7] Veyssman M E and Andreev N E 2015 J. Phys.: Conf. Ser. 653 012004
[8] Veyssman M, Röpke G, Winkel M and Reinholz H 2016 Phys. Rev. E 94 013203
[9] Sill V P 1965 Sov. Phys. JETP 20 1510–6
[10] Reinholz H and Röpke G 2012 Phys. Rev. E 85 036401
[11] Bornath T, Schlanges M, Hilse P, Kremp D and Bonitz M 2000 Laser Part. Beams 18 535–40
[12] Reinholz H 2005 Ann. Phys. Fr. 30 1–187
[13] Reinholz H, Redmer R, Röpke G and Wierling A 2000 Phys. Rev. E 62 5648
[14] Reinholz H, Röpke G, Rosmej S and Redmer R 2015 Phys. Rev. E 91 043105
[15] Mahan G D 2000 Many Particle Physics 3rd ed (New York: Plenum)
[16] Maksimov E G, Savrasov D Yu and Savrasov S Yu 1997 Phys. Usp. 40 337–58
[17] Veyssman M E, Agranat M B, Andreev N E, Ashitkov S I, Fortov V E, Khishchenko K V, Kostenko O F, Levashov P R, Ovchinnikov A V and Sitnikov D S 2008 J. Phys. B: At. Mol. Opt. Phys. 41 125704
[18] Abrikosov A A 1988 Fundamentals of the Theory of Metals (Amsterdam: North-Holland)
[19] Agranat M B, Andreev N E, Ashitkov S I, Veyssman M E, Levashov P R, Ovchinnikov A V, Sitnikov D S, Fortov V E and Khishchenko K V 2007 JETP Lett. 85 271–6