Second sum rule for the hot plasma permittivity

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Based on linear response theory, Kramers-Kronig relations, and diagram techniques of perturbation theory, it is shown that the second sum rule is satisfied for hot plasma permittivity. An explicit analytical expression for the second sum rule in the limit of weak nonideality is derived.

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Particular attention is paid to theoretical and experimental study of the frequency dependence of the plasma permittivity $\varepsilon(\omega)$ (see [1–5] and references therein). In this situation, of significant importance are exact relations for the permittivity $\varepsilon(\omega)$, which would make it possible to estimate the accuracy of the models used for describing the frequency dependence of the function $\varepsilon(\omega)$. Among such exact relations are the Kramers-Kronig relations (KKRs) and sum rules (see, e.g., [6,7]). As applied to the permittivity $\varepsilon(\omega)$ of homogeneous and isotropic plasma, which is defined as the long-wavelength limit of the longitudinal $\varepsilon^l(q,\omega)$ and transverse $\varepsilon^{tr}(q,\omega)$ permittivities [6],

$$\varepsilon(\omega)=\lim_{q\to 0}\varepsilon^l(q,\omega)=\lim_{q\to 0}\varepsilon^{tr}(q,\omega),\quad \varepsilon(\omega)=1+\frac{4\pi i}{\omega}\sigma(\omega), \tag{1}$$

the known sum rule is written as [6, 7]

$$\int_0^\infty \operatorname{Im}\varepsilon(\xi)\xi d\xi=\frac{\pi\omega_p^2}{2}, \tag{2}$$

where ω_p is the plasma frequency. In turn, KKRs for the permittivity $\varepsilon(\omega)$ of homogeneous and isotropic plasmas are written as [7] (see also [8])

$$\operatorname{Re}\varepsilon(\omega)=1+\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{+\infty}\left\{\operatorname{Im}\varepsilon(\xi)-\frac{4\pi\sigma_{\rm st}}{\xi}\right\}\frac{d\xi}{\xi-\omega}, \tag{3}$$

$$\operatorname{Im}\varepsilon(\omega)-\frac{4\pi\sigma_{st}}{\omega}=-\mathrm{P}\int_{-\infty}^{+\infty}\frac{\{\operatorname{Re}\varepsilon(\xi)-1\}}{\pi}\frac{d\xi}{\xi-\omega}, \tag{4}$$

where the symbol P before the integral signs in (3) and (4) means that the corresponding integral is understood as the principal-value integral, σ_{st} is the static conductivity of the plasma, defined as the static limit of the dynamic conductivity $\sigma(\omega)$ [Eq. (1)], $\sigma_{st}=\lim_{\omega\to 0}\sigma(\omega)$. In this case, for the function $\varepsilon(\omega)$, at real frequencies ω, the following equations [6, 7] are valid,

$$\operatorname{Re}\varepsilon(\omega)=\operatorname{Re}\varepsilon(-\omega),\ \operatorname{Im}\varepsilon(\omega)=-\operatorname{Im}\varepsilon(-\omega),\ \operatorname{Im}\varepsilon(\omega)>0\quad\text{for }\omega>0. \tag{5}$$

At the same time, according to (1), as shown in [9] based on linear response theory and diagram techniques of perturbation theory, the permittivity $\varepsilon(\omega)$ has the form

$$\varepsilon(\omega)=1-\frac{\omega_p^2}{\omega^2}-\frac{\varphi(\omega)}{\omega^2},\qquad \varphi(\omega)=\frac{4\pi}{3V}\langle\langle I^\beta|I^\beta\rangle\rangle_\omega, \tag{6}$$

$$I^\beta=\sum_a z_a e I_a^\beta,\quad I_a^\beta=\sum_{ps}\frac{\hbar p_\beta}{m_a}a_{ps}^\dagger a_{ps},$$
$$\omega_p=\left(\sum_a\frac{4\pi z_a^2e^2n_a}{m_a}\right)^{1/2}. \tag{7}$$

$$\langle\langle A|B\rangle\rangle_\omega\equiv-\frac{i}{\hbar}\int_0^{+\infty}\exp(i\omega t)\langle[A(t),B(0)]\rangle dt. \tag{8}$$

Here I^β is the total current operator, $A(t)$ is the operator A in the Heisenberg representation, the angular brackets $\langle\cdots\rangle$ mean averaging in the grand canonical ensemble with the exact Hamiltonian of the plasma, and $a_{ps}^\dagger$ and a_{ps} are the creation and annihilation operators for charged particles of type a with momentum $\hbar\mathbf{p}$ and spin number s, which are characterized by the charge z_ae, mass m_a, chemical potential μ_a, and average density of the number of particles n_a, so that the quasineutrality condition $\sum_a z_aen_a=0$ is satisfied. Relations (6)–(8) represent the permittivity in thermodynamic limit: $V\to\infty$, $N_a\to\infty$, $n_a=N_a/V=\text{const}$, where V is the plasma volume and N_a the total number of particles of a type. We note that relations (6)–(8) correspond to the known Kubo formula [10]. Integrating by parts in (6)–(8), it is easy to verify that [11]

$$\varepsilon(\omega)=1-\frac{\omega_p^2}{\omega^2}-\frac{m_2}{\omega^4}-\frac{\psi(\omega)}{\omega^4},$$
$$\psi(\omega)=\frac{4\pi}{3V}\left\langle\left\langle\frac{dI^\beta}{dt}\,\Big|\,\frac{dI^\beta}{dt}\right\rangle\right\rangle_\omega, \tag{9}$$

where m_2 is the so-called second moment of the high-frequency expansion for the function $\operatorname{Re}\varepsilon(\omega)$ [12],

$$m_2=\frac{4\pi}{3}\sum_{a\neq b}(n_an_b)^{1/2}\left\{\frac{z_az_be^2}{m_am_b}-\frac{z_a^2e^2}{m_a^2}\right\}\times\int\frac{d^3q}{(2\pi)^3}q^2u_{ab}(q)S_{ab}(q). \tag{10}$$

Here $u_{ab}(q)=\frac{4\pi z_az_be^2}{q^2}$ is the Fourier component of the Coulomb interparticle interaction potential, and $S_{ab}(q)$ is the static structure factor for particles of types a and b, which is directly related to the corresponding pair correlation

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function $g_{ab}(r)$,

$$S_{ab}(q) = \delta_{a,b} + (n_a n_b)^{1/2} \int \exp(i\mathbf{qr})\{g_{ab}(r) - 1\} d\mathbf{r}. \quad (11)$$

In turn, according to (3)–(5), we find [13]

$$\operatorname{Re}\varepsilon(\omega) = 1 - \frac{2}{\pi\omega^2}\int_0^\infty \operatorname{Im}\varepsilon(\xi)\xi d\xi - \frac{2}{\pi\omega^4} \times \int_0^\infty \operatorname{Im}\varepsilon(\xi)\xi^3 d\xi - \frac{\gamma^{(0)}(\omega)}{\omega^4}, \quad (12)$$

$$\gamma^{(0)}(\omega) = \frac{2}{\pi} P \int_0^\infty \frac{\operatorname{Im}\varepsilon(\xi)\xi^5 d\xi}{\omega^2 - \xi^2}. \quad (13)$$

Thus, if it could be proved that

$$\lim_{\omega\to\infty} \operatorname{Re}\psi(\omega) = 0, \quad \lim_{\omega\to\infty}\gamma^{(0)}(\omega) = 0, \quad (14)$$

not only would the validity of equality (2) immediately follow from the comparison of relations (9), (10) and (12), (13), but also the second sum rule for the permittivity $\varepsilon(\omega)$,

$$\int_0^\infty \operatorname{Im}\varepsilon(\xi)\xi^3 d\xi = \frac{\pi m_2}{2} \geqslant 0. \quad (15)$$

Let us perform a further consideration for a high-temperature two-component gas plasma consisting of electrons (subscript e) and ions (subscript i) in the parameter range

$$n_a\lambda_a^3 \ll 1,\ T \gg Ry,\ \lambda_a = \left(\frac{\hbar^2}{Tm_a}\right)^{1/2},\ Ry = \frac{m_e e^4}{2\hbar^2}, \quad (16)$$

where λ_a is the thermal de Broglie wavelength for particles of type a. The first condition in (16) corresponds to the transition to the quasiclassical description of an ideal plasma. The second condition in (16) corresponds to consideration of a fully ionized plasma in which one can neglect the bound states of electrons and ions (atoms and molecules; see, e.g., [14,16]). At the same time, the second inequality in (16) is equivalent to applicability of the Born approximation in quantum mechanics to the collisions of particles (see [16]). Consideration of the quantum effects is necessary, since the classical Coulomb system is unstable [16]. Therefore, if the conditions (16) are satisfied, the quasiclassical approximation and the weak nonideality approximation (or the integral smallness of the Coulomb interparticle interaction) can be used for description of the plasma [17].

Then, based on diagram techniques of perturbation theory [18], it can be shown that in the high frequency limit $\omega \gg \tilde{\nu}_{ei}$, where $\tilde{\nu}_{ei}$ is the characteristic frequency of electron-ion collisions, the function $\psi(\omega)$ is written as [11,17]

$$\psi(\omega) = -\frac{4\pi e^2 T}{3m_e^2}\int \frac{d^3q}{(2\pi)^3} q^3 |u_{ei}(q)|^2 \chi_{ee}^{(0)}(q,\omega)\chi_{ii}^{(0)}(q,0), \quad (17)$$

$$\chi_{ee}^{(0)}(q,\omega) = \frac{\Pi_{ee}^{RPA}(q,\omega)}{\varepsilon_{ee}^{RPA}(q,\omega)}, \quad \varepsilon_{ee}^{RPA}(q,\omega) = 1 - u_{ee}(q)\Pi_{ee}^{RPA}(q,\omega), \quad (18)$$

$$\chi_{ii}^{(0)}(q,0) = \frac{\Pi_{ii}^{RPA}(q,0)}{1 - u_{ii}^{eff}(q)\Pi_{ii}^{RPA}(q,0)}, \quad u_{ii}^{eff}(q) = u_{ii}(q) + |u_{ei}(q)|^2\chi_{ee}^{(0)}(q,0). \quad (19)$$

Here $\chi_{ee}^{(0)}(q,\omega)$ and $\varepsilon_{ee}^{RPA}(q,\omega)$ are, respectively, the "density-density" response function and dielectric function of the electron gas in the neutralized background of positive charge (collisionless approximation for plasma [15]), and $\chi_{ii}^{(0)}(q,0)$ is the static "density-density" response function for ions which interact with one another via the effective short-range potential $u_{ii}^{eff}(q)$ (19). This is easy to see in the case of Coulomb interaction $u_{ii}^{eff}(q) = u_{ii}(q)/\varepsilon_{ee}^{RPA}(q,0)$, i.e., when the ion-ion effective interaction is the Coulomb one, screened by electrons. Note that, in the classical limit ($\hbar \to 0$), the response function $\chi_{ii}^{(0)}(q,0)$ is determined in the appropriate approximation by the ion-ion static factor $S_{ii}(q)$ [Eq. (11)]: $T \lim_{\hbar\to 0}\chi_{ii}^{(0)}(q,0) = -n_i \lim_{\hbar\to 0} S_{ii}(q)$. In (18) and (19) $\Pi_{aa}^{RPA}(q,\omega)$ is the polarization operator in the random phase approximation (RPA) which in the quasiclassical case, when conditions (16) are satisfied, is given by [14]

$$\operatorname{Re}\Pi_{aa}^{RPA}(q,\omega) = -\frac{n_a}{\hbar qT}\left\{\left(\frac{m_a\omega}{q} + \frac{\hbar q}{2}\right) \times F_{1,1}\left(1,\frac{3}{2},-\frac{1}{2m_aT}\left(\frac{m_a\omega}{q} + \frac{\hbar q}{2}\right)^2\right) - \left(\frac{m_a\omega}{q} - \frac{\hbar q}{2}\right) \times F_{1,1}\left(1,\frac{3}{2},-\frac{1}{2m_aT}\left(\frac{m_a\omega}{q} - \frac{\hbar q}{2}\right)^2\right)\right\}, \quad (20)$$

$$\operatorname{Im}\Pi_{aa}^{RPA}(q,\omega) = -\frac{n_a}{2\hbar}\left(\frac{2\pi m_a}{Tq^2}\right)^{1/2} \times \left\{\exp\left[-\frac{1}{2m_aT}\left(\frac{m_a\omega}{q} - \frac{\hbar q}{2}\right)^2\right] - \exp\left[-\frac{1}{2m_aT}\left(\frac{m_a\omega}{q} + \frac{\hbar q}{2}\right)^2\right]\right\}. \quad (21)$$

$F_{1,1}(\alpha,\beta,x)$ is the degenerate hypergeometric function, and T is the system temperature. Relations (17)–(19) are valid within the adiabatic approximation for the ion subsystem ($m_i \gg z_i m_e$).

As is easy to show from (20),(21) the transition to the classical limit ($\hbar \to 0$) is equivalent to the conditions

$$\frac{\hbar^2q^2}{2m_a} \ll \hbar\omega \ll T, \quad \frac{\hbar^2q^2}{2m_a} \ll T \text{ (for } \omega = 0). \quad (22)$$

This means that consideration of a high frequency ω ($\omega \to \infty$), and a high value of the wave vector q ($q \to \infty$), which corresponds to small distances, the classical expressions for the frequency- and wave-vector-dependent correlation functions cannot be applied, although the conditions of the quasiclassical approximation are fulfilled [the first inequality in (16)]. Thus, the known Coulomb divergence in the kinetic theory of a classical plasma at small distances is conditioned by this circumstance (see, e.g., [15]). At the same time, according to (9), (10), and (17)

$$m_2 = -\psi(0) = \frac{4\pi e^2 T}{3m_e^2}\int \frac{d^3q}{(2\pi)^3} q^2 |u_{ei}(q)|^2 \chi_{ee}^{(0)}(q,0)\chi_{ii}^{(0)}(q,0). \quad (23)$$

Substituting (21) into (17)–(19), we can show [17] that

$$\operatorname{Im}\varepsilon(\omega\to\infty)\to\frac{C}{\omega^4\sqrt{\omega}},\quad \operatorname{Im}\psi(\omega\to\infty)\to-\frac{C}{\sqrt{\omega}},\quad C=\frac{2}{3}z_i\omega_p^4\left(\frac{Ry}{\hbar}\right)^{1/2}. \tag{24}$$

Let us pay attention to the fundamental necessity to consider quantum effects. Then, according to definition (9), the function $\psi(z)$ is an analytical function in the upper half plane of complex z ($\operatorname{Im} z>0$) and thereby [19] satisfies the KKRs. In this case, in contrast to the permittivity $\varepsilon(\omega)$ [see (3) and (4)], the function $\psi(\omega)$ has no singularity at $\omega=0$ [see (23)]. Thus, according to (3), (5), and (9) for the function $\operatorname{Re}\psi(\omega)$, in the limit $\omega\to\infty$ [see (14)] which is interesting, one can write

$$\operatorname{Re}\psi(\omega)=-\frac{2}{\pi}\mathrm{P}\int_0^\infty\frac{\operatorname{Im}\psi(\xi)\xi d\xi}{\omega^2-\xi^2}. \tag{25}$$

Taking into account (24), the passage to the limit $\omega\to\infty$ in (25) cannot be performed under the integral sign. In this case,

$$\mathrm{P}\int_0^\infty\frac{\operatorname{Im}\psi(\xi)\xi d\xi}{\omega^2-\xi^2}=\mathrm{P}\int_0^\infty\left\{\operatorname{Im}\psi(\xi)+\frac{C}{\sqrt{\xi}}\right\}\frac{\xi d\xi}{\omega^2-\xi^2}-C\mathrm{P}\int_0^\infty\frac{\sqrt{\xi}d\xi}{\omega^2-\xi^2}. \tag{26}$$

According to [20], for $\alpha>0$, $\beta>0$, and $0<\mu<2$, we have

$$\int_0^\infty\frac{x^{\mu-1}dx}{(\beta+x)(\alpha-x)}=\frac{\pi}{\alpha+\beta}[\beta^{\mu-1}\csc(\mu\pi)+\alpha^{\mu-1}\cot(\mu\pi)]. \tag{27}$$

For calculation of the last integral in the right-hand side of (26), let us use (27) for $\alpha=\beta=\omega$, $\mu=3/2$ and take into account that in the first integral in the right-hand side of (26) transition to the limit $\omega\to\infty$ can be performed under the integral sign. As a result, from (26) and (27) we obtain

$$\operatorname{Re}\psi(\omega\to\infty)\to\frac{\pi C}{2\sqrt{\omega}}. \tag{28}$$

A similar consideration can also be performed for the function $\gamma^{(0)}(\omega)$ [Eq. (13)] (see [13]). Thus, the validity of equalities (14) is proved. Hence, the hot plasma permittivity $\varepsilon(\omega)$ satisfies the second sum rule

$$\int_0^\infty\operatorname{Im}\varepsilon(\xi)\xi^3d\xi=\frac{2\pi^2e^2T}{3m_e^2}\int\frac{d^3q}{(2\pi)^3}q^2|u_{ei}(q)|^2\times\chi_{ee}^{(0)}(q,0)\chi_{ii}^{(0)}(q,0)\geqslant 0. \tag{29}$$

To calculate the integral on the right-hand side of (29), we will take into account that $\lim_{\omega\to 0}\operatorname{Im}\Pi_{aa}^{RPA}(q,\omega)=0$, and the static polarization operator $\Pi_{aa}^{RPA}(q,0)$, according to (20), is given by [21]

$$\Pi_{aa}^{RPA}(q,0)=-\frac{n_a}{T}\varphi(q\lambda_a),\quad \varphi(x)=F_{1,1}\left(1,\frac{3}{2},-\frac{x^2}{8}\right), \tag{30}$$

$$\lim_{x\to 0}\varphi(x)=1,\quad \lim_{x\to\infty}x^2\varphi(x)=4,\ 0<\varphi(x)<1,\quad \frac{d\varphi(x)}{dx}<0. \tag{31}$$

We note that the first equality in (31) corresponds to the classical limit for $\Pi_{aa}^{RPA}(q,0)$. Using (18), (19), and (29)–(31), it is easy to verify that

$$\int_0^\infty\operatorname{Im}\varepsilon(\xi)\xi^3d\xi=\frac{\sqrt{2}}{3}z_i\omega_p^4\left(\frac{Ry}{T}\right)^{1/2}M(\alpha_p,z_i,\theta),\quad \alpha_p=\frac{\hbar\omega_p}{T},\quad \theta=\left(\frac{m_e}{m_i}\right)^{1/2}, \tag{32}$$

$$M(\alpha_p,z_i,\theta)=\int_0^\infty\frac{x^2\varphi(x)\varphi(\theta x)dx}{x^2+\alpha_p^2\{\varphi(x)+z_i\varphi(\theta x)\}}. \tag{33}$$

Taking into account that $\theta\ll 1$, the dependence of the quantity $M(\alpha_p,z_i,\theta)$ on the parameter θ, according to (31), can be neglected,

$$M(\alpha_p,z_i,\theta)\cong M(\alpha_p,z_i,0)=\int_0^\infty\frac{x^2\varphi(x)dx}{x^2+\alpha_p^2\{\varphi(x)+z_i\}}, \tag{34}$$

$$\lim_{\alpha_p\to 0}M(\alpha_p,z_i,0)=M_0=\int_0^\infty\varphi(x)dx=\text{const}. \tag{35}$$

Thus, the second sum rule for the permittivity $\varepsilon(\omega)$ of hot plasma whose thermodynamic parameters satisfy conditions (16) and $\hbar\omega_p\ll T$ is written as

$$\int_0^\infty\operatorname{Im}\varepsilon(\xi)\xi^3d\xi=\frac{\sqrt{2}}{3}z_i\omega_p^4\left(\frac{Ry}{T}\right)^{1/2}M_0. \tag{36}$$

To estimate M_0 taking into account (31), we can use the approximation for the function $\varphi(x)=4(4+x^2)^{-1}$ [21]. In this case, $M_0=\pi$.

The results are essential for construction of self-consistent models of the frequency dispersion of the plasma permittivity $\varepsilon(\omega)$. In this case, a certain advantage of the second sum rule is associated with the dependence on the thermodynamic parameters of the plasma. Furthermore, by virtue of the asymptotic behavior of (24), the higher moments m_n $(n>2)$ of the permittivity $\varepsilon(\omega)$ diverge (see, e.g., [22]):

$$m_n=\int_0^\infty\operatorname{Im}\varepsilon(\xi)\xi^{2n-1}d\xi,\quad m_1=\frac{\pi\omega_p^2}{2},\quad m_2=\frac{\sqrt{2}}{3}z_i\omega_p^4\left(\frac{Ry}{T}\right)^{1/2}M_0,\quad m_{n>2}=\infty. \tag{37}$$

Thus, the sum rules for the hot nonrelativistic plasma permittivity $\varepsilon(\omega)$ are completely satisfied by the above results. In addition, when the quasiclassical conditions [see (16)] are fulfilled the quantum effects should be taken into account, since in this case the Coulomb divergence for small distances (large wave vectors) is absent. The divergence for small wave vectors (large distances) is canceled by the screening effect.

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