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Interaction of photons with plasmas and liquid metals—photoabsorption and scattering

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Abstract. Formulae for describing the photoabsorption and the photon scattering by a plasma or a liquid metal are derived in a unified manner. It is shown how the nuclear motion, the free-electron motion and the core-electron behaviour of each ion in the system determine the structure of the photoabsorption and scattering in an electron–ion mixture. The absorption cross section in the dipole approximation consists of three terms which represent the absorption caused by the nuclear motion, the absorption owing to the free-electron motion producing optical conductivity or inverse Bremsstrahlung and the absorption ascribed to the core-electron behaviour of each ion with the Doppler correction. Also, the photon scattering formula provides an analysis method for experiments observing the ion–ion dynamical structure factor (DSF), the electron–electron DSF giving plasma oscillations and the core-electron DSF yielding the x-ray Raman (Compton) scattering with a clear definition of the background scattering for each experiment, in a unified manner. A formula for anomalous x-ray scattering is also derived for a liquid metal. At the same time, Thomson scattering in plasma physics is discussed from this general point of view.

1. Introduction

For an isolated atom or the free-electron system without taking account of the existence of bound electrons, the theory of photoabsorption and scattering provides a simple formula, as given in the standard books [1]. However, in a real system such as a plasma or a liquid metal, photons are interacting with the free electrons and the bound electrons in the system: we must treat the free electrons and the bound electrons on an equal footing to investigate interactions of photons with matter. In some works treating plasmas [2–4], the absorption cross section $\sigma_a(\omega)$ is separated into three parts: $\sigma_{bb}(\omega)$, the absorption owing to the bound–bound transitions in the ion, $\sigma_{bf}(\omega)$, caused by the transitions from the bound to the free state, and $\sigma_{ff}(\omega)$ from the free–free transition, in the formula

$$\sigma_a(\omega) = \frac{4\pi\omega}{c} \Im \hat{\alpha}(\omega) \quad (1)$$

$$= \sigma_{bb}(\omega) + \sigma_{bf}(\omega) + \sigma_{ff}(\omega) \quad (2)$$

with use of the atomic polarizability $\hat{\alpha}(\omega)$. The situation is not so simple, as will be shown in this paper; photons interact with the nuclear motion through the bound electrons carried and the screening electrons, in addition to the ‘free’ electrons and the bound electrons in the system, in a coupled manner. Here, it should be mentioned that the free–free absorption in a plasma cannot be described by the same atomic polarizability $\hat{\alpha}(\omega)$ to give $\sigma_{bb}(\omega)$ and $\sigma_{bf}(\omega)$, as is shown in this paper. This example brings to light some confusions in treating the photon

interactions with plasmas. It is the purpose of this paper to clarify the mechanism of photon interactions with plasmas and liquid metals.

On the other hand, the experiments on photon scattering by matter are focused on the observation of either the nuclear motion, the free-electron motion or the core-electron behaviour of the ion by choosing the transferred momentum \mathbf{q} and energy ω suitable to the phenomena. Therefore, when the scattering by one of these motions is observed, the other motions yield the background scattering; there are many kinds of scattering called Raman, Rayleigh, Compton and Thomson, combined sometimes with the term ‘elastic’ and/or ‘inelastic’, for example, in a confused way. In this paper, we present the formula for scattering of photons by plasmas and liquid metals in a unified manner to show the nuclear motion, the free-electron motion and the core-electron behaviour of the ion; this formula can clarify the relationship between the observing scattering and the background scattering for each experiment, and provides the analysis method for each experiment.

The theory of photoabsorption in atomic systems is based on first-order time-dependent perturbation; the transition probability for the absorption of a photon (of wavevector \mathbf{q} and frequency ω with its polarization $e_{q\lambda}$) accompanied by a transition from a state ‘a’ to a state ‘b’ of the absorbing system provides the absorption cross section [5] in the form

$$\sigma_a(\mathbf{q}\lambda, \omega) = \frac{4\pi^2}{\hbar c \omega} \left(\frac{e}{m}\right)^2 \frac{1}{N} \sum_a p_a \sum_b \left| \langle b | \sum_{j=1}^{Z_A N} e_{q\lambda} \cdot \mathbf{p}_j e^{i\mathbf{q} \cdot \mathbf{r}_j} | a \rangle \right|^2 \delta\left(\frac{E_a - E_b}{\hbar} + \omega\right). \quad (3)$$

Here, a proper statistical averaging p_a over the initial states of the absorber has been performed; E_a is an eigenstate of the absorber (the nucleus–electron mixture). This expression can be rewritten by following the manner of Van Hove to derive the neutron scattering formula [6] in another form:

$$\sigma_a(\mathbf{q}\lambda, \omega) = \frac{4\pi^2 e^2}{\hbar c \omega} \frac{1}{2\pi N} \int_{-\infty}^{\infty} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} a(\mathbf{r}, t) d\mathbf{r} dt = \frac{4\pi^2 e^2}{\hbar c \omega} a(\mathbf{q}, \omega) \quad (4)$$

with

$$a(\mathbf{r}, t) \equiv e_{q\lambda} \int d\mathbf{r}' \langle \mathbf{j}(\mathbf{r}', 0) \mathbf{j}(\mathbf{r} + \mathbf{r}', t) \rangle \cdot e_{q\lambda} \quad (5)$$

in terms of the current operator of all electrons in the system consisting of N atoms with the atomic number Z_A :

$$\mathbf{j}(\mathbf{r}, t) \equiv \sum_{i=1}^{Z_A N} \delta(\mathbf{r} - \mathbf{r}_i(t)) \frac{\mathbf{p}_i(t)}{m}. \quad (6)$$

This means that the absorption cross section can be determined by the current–current correlation (dyad):

$$\mu_{JJ}(\mathbf{q}, \omega) = \frac{1}{N} \int e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} \langle \mathbf{j}(\mathbf{r}', 0) \mathbf{j}(\mathbf{r} + \mathbf{r}', t) \rangle d\mathbf{r}' dt \quad (7)$$

$$= \frac{1}{N} \int_{-\infty}^{\infty} \langle \mathbf{j}_q^*(0) \mathbf{j}_q(t) \rangle e^{-i\omega t} dt \quad (8)$$

with

$$\mathbf{j}_q(t) \equiv \sum_j \frac{\mathbf{p}_j(t)}{m} \exp[-i\mathbf{q} \cdot \mathbf{r}_j(t)]. \quad (9)$$

Therefore, the absorption cross section in the dipole approximation is obtained by taking the limit

$$\lim_{q \rightarrow 0} 2\pi a(\mathbf{q}, \omega) = \mu_{JJ}^L(0, \omega) \equiv \mu_{q=0}^{\text{tot}}(\omega) \quad (10)$$

where $a(q, \omega)$ reduces to the longitudinal current–current correlation $\mu_{JJ}^L(0, \omega)$, since the transverse current–current correlation $\mu_{JJ}^T(0, \omega)$ becomes identical with the longitudinal current–current correlation in this limit for the isotropic system.

On the other hand, when an incident photon state $\mathbf{k}_0, \mathbf{e}_0, \omega_0$ is scattered by a plasma to a state $\mathbf{k}_1, \mathbf{e}_1, \omega_1$, the differential scattering cross section is described in terms of the dynamical structure factor (DSF) $S_{ee}^{\text{tot}}(q, \omega)$ of all electrons involved in the plasma as free and bound electrons [5, 7] in the form

$$\frac{d^2\sigma}{d\Omega d\omega} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{Th}} \frac{k_1}{k_0} S_{ee}^{\text{tot}}(q, \omega) \quad (11)$$

with the Thomson cross section

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{Th}} \equiv \left(\frac{e^2}{mc^2} \right)^2 (\mathbf{e}_0 \cdot \mathbf{e}_1)^2. \quad (12)$$

Here, the total DSF is defined by

$$S_{ee}^{\text{tot}}(q, \omega) \equiv \frac{1}{2\pi N} \int e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} G_{ee}^{\text{tot}}(\mathbf{r}, t) d\mathbf{r} dt \quad (13)$$

in terms of the time-dependent density–density correlation function:

$$G_{ee}^{\text{tot}}(\mathbf{r}, t) \equiv \int d\mathbf{r}' \langle \rho_e(\mathbf{r}', 0) \rho_e(\mathbf{r} + \mathbf{r}', t) \rangle \quad (14)$$

with

$$\rho_e(\mathbf{r}, t) \equiv \sum_{j=1}^{Z_A N} \delta(\mathbf{r} - \mathbf{r}_j(t)). \quad (15)$$

The above expressions for the absorption cross section (4) and the scattering cross section (11) are written for all electrons, which are contained as the bound electrons or the free electrons coupled with N nuclei with the atomic number Z_A in the system. These expressions are only formal, and do not give any information about the mechanism of the photoabsorption and scattering in a real system. Under the assumption that a plasma or a liquid metal clearly consists of ions with the charge Z_f and free electrons, we give the physical structure for the absorption cross section from (4) in section 2, and for the scattering cross section from (11) in section 3. The last section is devoted to conclusions. A glossary of main symbols is given as table 1.

2. Photoabsorption

We can obtain the absorption cross section in the dipole approximation (10) from the dynamical structure factor $S_{ee}^{\text{tot}}(q, \omega)$ of the total electrons by noting the following relation [8, 9]:

$$\mu_q^{\text{tot}}(\omega) \equiv \frac{1}{N} \int_{-\infty}^{\infty} \langle \mathbf{j}_q^*(0) \mathbf{j}_q(t) \rangle_L e^{-i\omega t} dt = 2\pi \frac{\omega^2}{q^2} S_{ee}^{\text{tot}}(q, \omega) \quad (16)$$

where the ‘total electrons’ are all electrons contained in the system as the core electrons around each nucleus and the free electrons. From the definition of the DSF

$$S_{ee}^{\text{tot}}(q, \omega) \equiv \frac{1}{2\pi N} \int_{-\infty}^{\infty} I^{\text{tot}}(q, t) e^{i\omega t} dt \quad (17)$$

in terms of the intermediate scattering function

$$I^{\text{tot}}(q, t) \equiv \langle \rho_e(\mathbf{q}, t) \rho_e^*(\mathbf{q}, 0) \rangle \quad (18)$$

Table 1. A glossary of main symbols: a list of notation and an equation to define each symbol (in the column headed ‘Definitions’).

| Symbols | Definitions | Meanings |
|---|--------------|---|
| a_q^\dagger, a_q | | Creation and annihilation operators |
| $C_{\text{el}}(q) = C_{\text{el}}(q, 0)$ | | Electron–ion direct correlation function |
| $\mathbf{d}(t)$ | (A.8) | Dipole moment |
| $\mathbf{e}_{q\lambda}, \mathbf{e}_0, \mathbf{e}_1$ | | Polarization of a photon |
| $f_1(q), f_A(q)$ | (31) | Ionic and atomic form factors |
| $f_{lm}(q) \equiv \langle l \exp[i\mathbf{q} \cdot \mathbf{r}] m \rangle$ | | James’s symbol [16] |
| $G(q, \omega), G(q) = G(q, 0)$ | | Dynamical and static local-field correction |
| $G_{\text{ee}}^{\text{tot}}(\mathbf{r}, t)$ | (14) | Time-dependent density correlation of total electrons |
| $k(\omega)$ | (A.16) | Absorption coefficient |
| N | | The total nucleus (ion) number in the system |
| $S_{\text{ee}}^{\text{tot}}(q, \omega)$ | (52) | DSF of the total electrons in the system |
| $S_{\text{ee}}(q, \omega), S_{\text{el}}(q, \omega), S_{\text{II}}(q, \omega)$ | (74), (39) | DSFs for the electron–ion mixture |
| $S_{\text{s}}(q, \omega)$ | (56) | Self-part of $S_{\text{II}}(q, \omega)$ |
| $\tilde{S}^{\text{ce}}(q, \omega), S^{\text{ce}}(q, \omega)$ | (36) | DSF of the core electrons in the ion |
| $S_{\text{ee}}^0(q, \omega)$ | (42) | ‘Free’-electron DSF |
| $S_{\text{inc}}^{\text{I}}(q), S_{\text{inc}}^{\text{A}}(q)$ | (67) | Incoherent Compton scattering caused by the ion and atom |
| $Z_A = Z_B + Z_{\text{f}}$ | | The atomic number (bound and free electrons) |
| $\hat{\alpha}(\omega), \hat{\alpha}^{\text{ce}}(\omega)$ | (51), (A.11) | Atomic polarizability |
| $\mu_{JJ}(q, \omega)$ | (7) | Current–current correlation for the total electrons |
| $\mu_q^{\text{tot}}(\omega) \equiv \mu_{JJ}^{\text{L}}(q, \omega)$ | (16) | Longitudinal part of μ_{JJ} proportional to $\sigma_a(\omega)$ |
| $\mu_q^{\text{nuc}}(\omega), \mu_q^{\text{fe}}(\omega), \mu_q^{\text{ce}}(\omega)$ | | Nucleus, free- and core-electron contributions to $\mu_q^{\text{tot}}(\omega)$ |
| $\rho(q) = \rho(q, 0)$ | (41), (78) | Free-electron cloud in the pseudoatom |
| $\rho_{\text{e}}(\mathbf{q}, t) \equiv \rho_{\text{c}}(\mathbf{q}, t) + \rho_{\text{f}}(\mathbf{q}, t)$ | (19) | Total electron distribution (the core and free electrons) |
| $\rho_{\text{B}}(\mathbf{q}, t), \delta\rho_{\text{B}}(\mathbf{q}, t)$ | (32), (37) | Bound-electron distribution in the ion and its deviation |
| $\rho_{\text{I}}(\mathbf{q}, t)$ | (23) | The ion (nucleus) distribution |
| $\sigma_a(q\lambda, \omega), \sigma_a(\omega) = \sigma_a(0, \omega)$ | (3) | Absorption cross section of a photon state $(q, \omega, \mathbf{e}_{q\lambda})$ |
| $\hat{\sigma}_{\text{L}}^{\text{ce}}(\omega), \hat{\sigma}_{\text{L}}^{\text{fe}}(\omega)$ | (A.14) | Conductivities of core and free electrons |
| $\chi_q^{0\text{e}}$ | | Density response function of non-interacting electron gas |
| $\chi_q^{\text{tot}}[\omega], \chi_q^{\text{fe}}[\omega], \chi_q^{\text{ce}}[\omega]$ | (76), (A.12) | Density responses of total, free and core electrons |

we can determine the total DSF in terms of the total electron density $\rho_{\text{e}}(\mathbf{q}, t)$ from $I^{\text{tot}}(q, t)$. Here, note that the total electron density can be split into the core-electron part $\rho_{\text{c}}(\mathbf{q}, t)$ and the free-electron part $\rho_{\text{f}}(\mathbf{q}, t)$:

$$\rho_{\text{e}}(\mathbf{q}, t) \equiv \sum_{k=1}^{Z_A N} \exp[i\mathbf{q} \cdot \mathbf{r}_k(t)] \quad (19)$$

$$= \rho_{\text{c}}(\mathbf{q}, t) + \rho_{\text{f}}(\mathbf{q}, t). \quad (20)$$

Furthermore, the core electrons are considered to be distributed among nuclei with positions \mathbf{R}_α :

$$\rho_c(\mathbf{q}, t) \equiv \sum_{\alpha=1}^N \sum_{j=1}^{Z_B} \exp[i\mathbf{q} \cdot \mathbf{r}_{j\alpha}(t)] = \sum_{\alpha=1}^N \sum_{j=1}^{Z_B} \exp[i\mathbf{q} \cdot (\mathbf{r}'_{j\alpha}(t) + \mathbf{R}_\alpha(t))] \quad (21)$$

$$= \sum_{\alpha=1}^N \left(\sum_{j=1}^{Z_B} \exp[i\mathbf{q} \cdot \mathbf{r}'_{j\alpha}(t)] \right) \exp[i\mathbf{q} \cdot \mathbf{R}_\alpha(t)] \quad (22)$$

which can be approximated by using the form factor $f_1(q)$ of the Z_B core electrons as follows:

$$\rho_c(\mathbf{q}, t) \simeq \left\langle \sum_{j=1}^{Z_B} \exp[i\mathbf{q} \cdot \mathbf{r}'_{j0}(t)] \right\rangle \sum_{\alpha=1}^N \exp[i\mathbf{q} \cdot \mathbf{R}_\alpha(t)] \equiv f_1(q) \rho_1(\mathbf{q}, t). \quad (23)$$

With the use of this approximation, we obtain the intermediate scattering function

$$I^{\text{tot}}(q, t) \equiv \langle [\rho_c(\mathbf{q}, t) + \rho_f(\mathbf{q}, t)] [\rho_c^*(\mathbf{q}, 0) + \rho_f^*(\mathbf{q}, 0)] \rangle \quad (24)$$

$$= \langle \rho_c(\mathbf{q}, t) \rho_c^*(\mathbf{q}, 0) \rangle + \langle \rho_f(\mathbf{q}, t) \rho_c^*(\mathbf{q}, 0) \rangle + \langle \rho_c(\mathbf{q}, t) \rho_f^*(\mathbf{q}, 0) \rangle \\ + \langle \rho_f(\mathbf{q}, t) \rho_f^*(\mathbf{q}, 0) \rangle \quad (25)$$

$$= N |f_1(q)|^2 F_{\text{II}}(q, t) + N [Z_B F^{\text{ce}}(q, t) - |f_1(q)|^2] F_s(q, t) \\ + N Z_f F_{\text{ee}}(q, t) + 2N \sqrt{Z_f} f_1(q) F_{\text{el}}(q, t). \quad (26)$$

In the above, several correlations among free electrons and ions are defined as follows:

$$F_{\text{II}}(q, t) \equiv \sum_{\alpha, \beta} \langle \exp[i\mathbf{q} \cdot (\mathbf{R}_\alpha(t) - \mathbf{R}_\beta(0))] \rangle / N \quad (27)$$

$$F_s(q, t) \equiv \langle \exp[i\mathbf{q} \cdot (\mathbf{R}_\alpha(t) - \mathbf{R}_\alpha(0))] \rangle \quad (28)$$

$$F_{\text{ee}}(q, t) \equiv \langle \rho_f(\mathbf{q}, t) \rho_f^*(\mathbf{q}, 0) \rangle / (Z_f N) \quad (29)$$

$$F_{\text{el}}(q, t) \equiv \langle \rho_1(\mathbf{q}, t) \rho_f^*(\mathbf{q}, 0) \rangle / (\sqrt{Z_f} N) \quad (30)$$

and the ionic form factor in (23) is defined for the core electrons in the ion in a plasma by

$$f_1(q) \equiv \langle \rho_B(\mathbf{q}, t) \rangle \quad (31)$$

with the bound-electron density around α -nucleus:

$$\rho_B(\mathbf{q}, t) \equiv \sum_{j=1}^{Z_B} \exp[i\mathbf{q} \cdot \mathbf{r}'_{j\alpha}(t)] = \sum_{j=1}^{Z_B} \exp[i\mathbf{q} \cdot \mathbf{r}'_{j0}(t)] \quad (32)$$

which becomes identical with the bound-electron density of any nucleus ($\alpha = 0$). Also, the electron–electron correlation between the core electrons in the ion is defined by

$$Z_B F^{\text{ce}}(q, t) \equiv \langle \rho_B(\mathbf{q}, t) \rho_B^*(\mathbf{q}, 0) \rangle. \quad (33)$$

From equation (26), we can represent the total electron DSF in terms of the ion–ion DSF $S_{\text{II}}(q, \omega)$, the electron–ion DSF $S_{\text{el}}(q, \omega)$ and the electron–electron DSF $S_{\text{ee}}(q, \omega)$ in the form

$$S_{\text{ee}}^{\text{tot}}(q, \omega) \equiv \frac{1}{2\pi N} \int_{-\infty}^{\infty} I^{\text{tot}}(q, t) e^{i\omega t} dt \\ = |f_1(q)|^2 S_{\text{II}}(q, \omega) + 2\sqrt{Z_f} f_1(q) S_{\text{el}}(q, \omega) + Z_f S_{\text{ee}}(q, \omega) \\ + Z_B \int \tilde{S}^{\text{ce}}(q, \omega - \omega') S_s(q, \omega') d\omega'. \quad (34)$$

Also, the DSF for the core electrons in each ion is defined as

$$\tilde{S}^{\text{ce}}(q, \omega) \equiv S^{\text{ce}}(q, \omega) - |f_I(q)|^2 \delta(\omega) / Z_B \quad (35)$$

$$= \frac{1}{2\pi Z_B} \int_{-\infty}^{\infty} \langle \delta\rho_B(\mathbf{q}, t) \delta\rho_B^*(\mathbf{q}, 0) \rangle e^{i\omega t} dt \quad (36)$$

with the use of the density deviation $\delta\rho_B(\mathbf{q}, t)$ from its average $\langle \rho_B(\mathbf{q}, t) \rangle$:

$$\delta\rho_B(\mathbf{q}, t) \equiv \rho_B(\mathbf{q}, t) - \langle \rho_B(\mathbf{q}, t) \rangle. \quad (37)$$

With the help of the following relations derived in the previous work [10]:

$$S_{\text{ee}}(q, \omega) = \frac{|\rho(q)|^2}{Z_f} S_{\Pi}(q, \omega) + S_{\text{ee}}^0(q, \omega) \quad (38)$$

$$S_{\text{el}}(q, \omega) = \frac{\rho(q)}{\sqrt{Z_f}} S_{\Pi}(q, \omega) \quad (39)$$

the DSF (34) of the total of the electrons is written as

$$S_{\text{ee}}^{\text{tot}}(q, \omega) = |f_I(q) + \rho(q)|^2 S_{\Pi}(q, \omega) + Z_f S_{\text{ee}}^0(q, \omega) + Z_B \int \tilde{S}^{\text{ce}}(q, \omega - \omega') S_s(q, \omega') d\omega'. \quad (40)$$

Here, $\rho(q)$ represents the Fourier transforms of the electron cloud $\rho(r)$ forming a neutral pseudoatom screening the ion:

$$\rho(q) \equiv n_0^{\text{e}} C_{\text{el}}(q) \chi_q^{0\text{e}} / \{1 + n_0^{\text{e}} \beta v_{\text{ee}}(q) [1 - G(q)] \chi_q^{0\text{e}}\} \quad (41)$$

which is exactly as prescribed by the use of the electron-ion direct correlation function $C_{\text{el}}(q)$ and the local-field correction (LFC) $G(q)$ [10]. Also, $S_{\text{ee}}^0(q, \omega)$ has the same form as the DSF in the jellium model except that the dynamical LFC $G(q, \omega)$ should be determined for an electron-ion mixture not in the jellium model, as written in the form

$$S_{\text{ee}}^0(q, \omega) \equiv -\frac{1}{\pi} \frac{1}{n_0^{\text{e}} v_{\text{ee}}(q)} \frac{\hbar\beta}{1 - \exp(-\beta\hbar\omega)} \Im \left(\frac{1}{\tilde{\epsilon}(q, \omega)} \right) \quad (42)$$

with

$$\tilde{\epsilon}(q, \omega) \equiv 1 + n_0^{\text{e}} \beta v_{\text{ee}}(q) \frac{\chi_q^{0\text{e}}[\omega]}{1 - n_0^{\text{e}} \beta v_{\text{ee}}(q) G(q, \omega) \chi_q^{0\text{e}}[\omega]} \quad (43)$$

which is also an exact (but formal) expression for the ‘free’-electron DSF. To take account of the absorption due to the motion of nuclei, we must add the nucleus charge current in (9) as $e\mathbf{j} = e(\mathbf{j}_{\text{e}} - Z_A \mathbf{j}_{\text{N}})$ with

$$\mathbf{j}_{\text{N}} \equiv \sum_{\alpha} \frac{P_{\alpha}}{M} \delta(\mathbf{r} - \mathbf{R}_{\alpha}).$$

This contribution can be taken by calculating the following charge correlation:

$$e^2 I^{\text{tot+nuc}}(q, t) \equiv e^2 \langle [\rho_{\text{e}}(q, t) - Z_A \rho_{\text{N}}(q, t)] [\rho_{\text{e}}^*(q, 0) - Z_A \rho_{\text{N}}^*(q, 0)] \rangle \quad (44)$$

with

$$\rho_{\text{N}}(q, t) = \sum_{\alpha} \exp[i\mathbf{q} \cdot \mathbf{R}_{\alpha}(t)].$$

Thus, we obtain the final expression for deriving the photoabsorption cross section:

$$I_{\text{ee}}^{\text{tot+nuc}}(q, \omega) / N = |f_I(q) + \rho(q) - Z_A|^2 S_{\Pi}(q, \omega) + Z_f S_{\text{ee}}^0(q, \omega) + Z_B \int \tilde{S}^{\text{ce}}(q, \omega - \omega') S_s(q, \omega') d\omega' \quad (45)$$

which with the aid of (16) leads finally to the expression for the absorption cross section:

$$\mu_q^{\text{tot}}(\omega) = |f_1(q) + \rho(q) - Z_A|^2 \mu_q^{\text{nuc}}(\omega) + Z_I \mu_q^{\text{fe}}(\omega) + Z_B \int \mu_q^{\text{ce}}(\omega - \omega') S_s(q, \omega') d\omega'. \quad (46)$$

The absorption cross section $\mu_q^{\text{ce}}(\omega)$ owing to the core electrons involved in the third term in (46) provides the standard expression for the photoabsorption cross section in terms of the dipole–dipole correlation, the atomic polarizability $\hat{\alpha}(\omega)$ or the longitudinal conductivity $\hat{\sigma}_L^{\text{ce}}(\omega)$:

$$Z_B e^2 \mu_{q=0}^{\text{ce}}(\omega) \equiv \lim_{q \rightarrow 0} \int_{-\infty}^{\infty} \langle e j_q^{\text{ce}*}(0) e j_q^{\text{ce}}(t) \rangle_L e^{-i\omega t} dt \quad (47)$$

$$= \frac{\omega^2}{3} \int_{-\infty}^{\infty} \langle \mathbf{d}(0) \cdot \mathbf{d}(t) \rangle e^{-i\omega t} dt \quad (48)$$

$$= \frac{2\hbar\omega^2}{1 - \exp(-\beta\hbar\omega)} \Im \hat{\alpha}^{\text{ce}}(\omega) \quad (49)$$

$$= \frac{2\hbar\omega}{1 - \exp(-\beta\hbar\omega)} \Re \hat{\sigma}_L^{\text{ce}}(\omega) \quad (50)$$

with the definition of the atomic polarizability in terms of the density–density response function of the core electrons in the ion:

$$\hat{\alpha}^{\text{ce}}(\omega) \equiv -e^2 \int \int z \chi^{\text{ce}}(\mathbf{r}, \mathbf{r}'; \omega) z' d\mathbf{r} d\mathbf{r}'. \quad (51)$$

These expressions can be obtained from (16) and the general relation [8] among the DSF $S_{\text{ce}}^{\text{tot}}(q, \omega)$, the density–density response function $\chi_q^{\text{tot}}[\omega]$ and the longitudinal conductivity $\sigma_L^{\text{tot}}[q, \omega]$ as follows (see appendix A):

$$S_{\text{ce}}^{\text{tot}}(q, \omega) \equiv \frac{1}{2\pi N} \int_{-\infty}^{\infty} \langle \rho_{\text{e}}(\mathbf{q}, t) \rho_{\text{e}}^*(\mathbf{q}, 0) \rangle e^{i\omega t} dt \quad (52)$$

$$= -\frac{\hbar}{1 - \exp(-\beta\hbar\omega)} \frac{1}{\pi} \Im \chi_q^{\text{tot}}[\omega] \quad (53)$$

$$= \frac{\hbar}{1 - \exp(-\beta\hbar\omega)} \frac{q^2}{\pi\omega} \Re \sigma_L^{\text{tot}}[q, \omega]. \quad (54)$$

In this way, the absorption cross section (4) owing to the core electrons contained in each ion in a plasma can be written in the dipole approximation in several forms:

$$\sigma_a^{\text{ce}}(0, \omega) = \frac{4\pi\omega}{c} \frac{1}{1 - \exp(-\beta\hbar\omega)} \Im \hat{\alpha}^{\text{ce}}(\omega) \quad (55a)$$

$$= \frac{4\pi}{c} \frac{1}{1 - \exp(-\beta\hbar\omega)} \Re \hat{\sigma}_L^{\text{ce}}(\omega) \quad (55b)$$

$$= 4\pi^2 \frac{e^2}{\hbar c} \omega \frac{1}{2\pi} \int \frac{\langle \mathbf{d}(0) \cdot \mathbf{d}(t) \rangle}{3e^2} e^{-i\omega t} dt \quad (55c)$$

$$= 4\pi^2 \frac{e^2}{\hbar c} \omega \sum_{ab} p_a |\langle b | z^{\text{ce}} | a \rangle|^2 \delta\left(\frac{E_b - E_a}{\hbar} - \omega\right) \quad (55d)$$

with

$$z^{\text{ce}} \equiv \sum_{j=1}^{Z_B} z_j$$

for incident photons polarized in the z -direction. In the works [2–4] treating high-temperature plasmas, the factor $[1 - \exp(-\beta\hbar\omega)]^{-1}$ in (55a) is omitted; this omission leads to the definition of the *net absorption* cross section [2].

In the third term, the self-part of the ionic DSF for the high-frequency region [9]

$$S_s(q, \omega) = \frac{1}{2\pi} \frac{1}{v_T q} \exp \left[-\frac{1}{2} \left(\frac{\omega}{v_T q} \right)^2 \right] \quad (56)$$

gives rise to the Doppler correction to the atomic photoabsorption; when a photon with a momentum $\hbar q_0 \equiv \hbar|\omega_0 - \omega_1|/c$ is absorbed, associated with the transition between two bound levels with a frequency difference $|\omega_0 - \omega_1|$, the third term becomes

$$\int \mu_{q_0}^{\text{ce}}(\omega - \omega') S_s(q_0, \omega') d\omega' \approx \int \mu_{q=0}^{\text{ce}}(\omega - \omega') \frac{1}{\sqrt{\pi} \omega_D} \exp \left[-\left(\frac{\omega'}{\omega_D} \right)^2 \right] d\omega' \quad (57)$$

where the Doppler width ω_D is given by $\omega_D \equiv |\omega_0 - \omega_1| \sqrt{2} v_T / c$ with $v_T^2 \equiv kT/m$.

Since the absorption cross section $\mu_{q=0}^{\text{ce}}(\omega)$ is derived for the nucleus–electron mixture, this can be written in the form for treating the Stark effect [11]:

$$Z_B e^2 \mu_{q=0}^{\text{ce}} = \frac{\omega^2}{3} \int_{-\infty}^{\infty} \langle \mathbf{d}(0) \cdot \mathbf{d}(t) \rangle e^{-i\omega t} dt = \frac{\omega^2}{3} \int e^{-i\omega t} dt \int d\epsilon q(\epsilon) \langle \mathbf{d}(0) \cdot \mathbf{d}(t) \rangle_{\epsilon} \quad (58)$$

using the microfield distribution $q(\epsilon) = \langle \delta(\epsilon - \mathbf{E}_i) \rangle$. This expression (58) gives a formula for treating the Stark broadening in a plasma [12].

The second term of (46) represents the absorption owing to the free electrons:

$$Z_f e^2 \mu_{q=0}^{\text{fe}}(\omega) = \frac{2\hbar\omega Z_f}{1 - \exp(-\beta\hbar\omega)} \Re \hat{\sigma}_L^{\text{fe}}(\omega) \quad (59)$$

which can be approximated by the Drude model using the frequency-dependent collision frequency $\nu(\omega)$:

$$4\pi \sigma_L^{\text{fe}}(\omega) \equiv 4\pi Z_f n_1 \hat{\sigma}_L^{\text{fe}}(\omega) \simeq \omega_p^2 / [\nu(\omega) - i\omega]. \quad (60)$$

Thus, the absorption coefficient $\kappa(\omega) = 4\pi \Re \sigma_L(\omega) / [n(\omega)c]$ owing to the free electrons is written as

$$4\pi \Re \sigma_L^{\text{fe}}(\omega) = \begin{cases} \frac{\sigma_0}{[\omega/\nu(0)]^2 + 1} & \text{for } \omega \lesssim \omega_p \\ \left(\frac{\omega_p}{\omega} \right)^2 \nu(\omega) & \text{for } \omega \gg \omega_p \end{cases} \quad (61)$$

with $\sigma_0 = \omega_p^2 / [4\pi \nu(0)]$ denoting the dc conductivity and ω_p denoting the plasma frequency. The upper alternative of (61) provides the optical conductivity as was observed in the case of liquid Na [13], and the lower one yields the inverse Bremsstrahlung [14]:

$$k(\omega) = \left(\frac{\omega_p}{\omega} \right)^2 \frac{\nu(\omega)}{n(\omega)c} = \frac{\omega_p^2 \nu(\omega)}{c\omega \sqrt{\omega^2 - \omega_p^2}} \quad (62)$$

with the refractive index $n(\omega)$ (see appendix A).

The first term of the absorption cross section (46) represents the absorption owing to the nuclear motion, which becomes zero in this approximation, since $f_1(0) = Z_B$ and $\rho(0) = Z_f$; the nucleus with the charge Z_A is perfectly neutralized by the bound electrons $f_1(r)$ and the free-electron cloud $\rho(r)$. It should be noticed that some part $\rho(q)$ of the free-electron contribution to the absorption is involved in the nuclear motion due to the relation (38), which means that the electron cloud $\rho(r)$ is attached to each nucleus together with the bound electrons $f_1(r)$, and the other part contributes to the free-electron absorption as given by (59).

3. Photon scattering

As we have proven in the previous section, the photon scattering can be described by the DSF $S_{ee}^{\text{tot}}(q, \omega)$ of all electrons in the system:

$$I(q, \omega)/N = S_{ee}^{\text{tot}}(q, \omega) = |f_I(q) + \rho(q)|^2 S_{II}(q, \omega) + Z_f S_{ee}^0(q, \omega) + Z_B \int \tilde{S}^{\text{ce}}(q, \omega - \omega') S_s(q, \omega') d\omega'. \quad (63)$$

This expression contains three dynamic structure factors: the ion-ion DSF $S_{II}(q, \omega)$, which is observed usually in thermal neutron scattering experiments, the core-electron DSF $\tilde{S}^{\text{ce}}(q, \omega)$ defined by (36) and the ‘free’-electron DSF $S_{ee}^0(q, \omega)$ defined by (42).

For the purpose of presenting the inelastic x-ray scattering for an incident photon with energy $\hbar\omega_0 \gg I$ (the ionization energy), equation (63) is rewritten in a form that focuses on $S_{II}(q, \omega)$:

$$I(q, \omega)/N = |f_I(q) + \rho(q)|^2 S_{II}(q, \omega) + Z_f S_{ee}^0(q, \omega) + Z_B S_{\text{inc}}^I(q, \omega) \quad (64)$$

with

$$Z_B S_{\text{inc}}^I(q, \omega) \equiv Z_B \int \tilde{S}^{\text{ce}}(q, \omega - \omega') S_s(q, \omega') d\omega' \simeq Z_B \tilde{S}^{\text{ce}}(q, 0). \quad (65)$$

On the basis of this equation, the dynamic structure factors $S_{II}(q, \omega)$ for liquid metals were observed by Sinn *et al* [15] by means of inelastic x-ray scattering. In this experiment, the second and third terms are regarded as yielding the incoherent scattering from the free and bound electrons.

The x-ray diffraction from a liquid metal or a plasma is described by the static structure factor $S_{ee}^{\text{tot}}(q)$:

$$S_{ee}^{\text{tot}}(q) = \int S_{ee}^{\text{tot}}(q, \omega) d\omega = |f_I(q) + \rho(q)|^2 S_{II}(q) + Z_f S_{ee}^0(q) + Z_B S_{\text{inc}}^I(q) \quad (66)$$

which is an extension of the usual formula for x-ray diffraction [16] to the case of the metallic system [10]. Here, $Z_B S_{\text{inc}}^I(q)$ denotes the incoherent Compton scattering produced by the bound electrons in each ion:

$$Z_B S_{\text{inc}}^I(q) = Z_B \tilde{S}^{\text{ce}}(q) \equiv \langle \delta\rho_B(q) \delta\rho_B^*(q) \rangle = Z_B S^{\text{ce}}(q) - |f_I(q)|^2 \quad (67)$$

$$\approx Z_B - \sum_{jk} |f_{jk}(q)|^2 \quad (68)$$

which can be evaluated approximately using the formula given by James [16] in terms of $f_{lm}(q) \equiv \langle l | \exp[i\mathbf{q} \cdot \mathbf{r}] | m \rangle$, and $S_{ee}^0(q)$ is the ‘free’-electron structure factor. Here, it should be noticed that equation (67) provides a formula for evaluating a more accurate incoherent scattering (even for a plasma), compared to James’s expression (68), and can be used for the analysis of the x-ray diffraction to obtain a more exact result. For a liquid metal or a plasma, the incoherent Compton scattering $Z_A S_{\text{inc}}^A(q)$ in the system consisting of neutral atoms is replaced by

$$Z_A S_{\text{inc}}^A(q) \approx Z_A - \sum_{jk} |f_{jk}(q)|^2 \quad (69)$$

$$\Rightarrow Z_B S_{\text{inc}}^I(q) + Z_f S_{ee}^0(q) \quad (70)$$

in conjunction with the replacement of the atomic form factor: $f_A(q) \Rightarrow f_I(q) + \rho(q)$. Since $f_A(q) \simeq f_I(q) + \rho(q)$ [17, 18], the x-ray diffraction experiment on a liquid metal can be

analysed by using the atomic form factor $f_A(q)$ as if the liquid metal is a non-metallic system. Moreover, on the basis of (66), Nardi *et al* [19] have proposed using x-ray scattering as a diagnostic for dense strongly coupled plasmas; the possibility of obtaining information on the electron-ion temperature relaxation time as well as a temperature diagnostic is indicated in addition to an equation-of-states diagnostic.

The ‘free’-electron DSF $S_{ee}^0(q, \omega)$ in (63) becomes the electron DSF $S_{ee}^{\text{jell}}(q, \omega)$ in the jellium model if the dynamical LFC $G(q, \omega)$ in (42) is approximated by the dynamical LFC $G^{\text{jell}}(q, \omega)$ of the jellium model. In this sense, the inelastic x-ray scattering experiments [20–22] for $\omega \sim \omega_p$ provide the DSF of the electron gas in a metal. However, it should be remembered that $S_{ee}^0(q, \omega)$ is only a part of the electron DSF given by (38). For large energy transfer $\omega \gg \omega_p$, this term produces Compton scattering due to the free electrons [23].

Inelastic x-ray scattering by the core electrons in the ion [24–26] is described by the core-electron DSF $\tilde{S}^{\text{ce}}(q, \omega)$ involved in (63). This inelastic x-ray scattering discriminates between Raman and Compton scattering according to the incoming photon energy compared with the ionization energy. It should be noticed that the Raman scattering cross section is closely related to the photoabsorption cross section, since the DSF $\tilde{S}^{\text{ce}}(q, \omega)$ has a relation to the longitudinal current-current correlation $\mu_q^{\text{ce}}(\omega)$, giving the absorption cross section as (16) shows. In the inelastic x-ray experiments, where the transfer energy ω is chosen as suitable for the determination of $\tilde{S}^{\text{ce}}(q, \omega)$ or $S_{ee}^0(q, \omega)$ in (63), the first term of (63) provides elastic scattering called Rayleigh scattering [27], since the ion-ion DSF can be treated as $S_{II}(q, \omega) \sim S_{II}(q)\delta(\omega)$ for this ω -range.

Note that the inelastic scattering formula (63) for x-rays is only applicable to the non-resonant case ($\omega_0 \gg I$) where the incident x-ray energy ω_0 is far from the ionization energy I . When we treat anomalous x-ray scattering ($\omega_0 \lesssim I$) or light (and electromagnetic wave) scattering to observe the ion-ion DSF $S_{II}(q, \omega)$, we must take into account the second-order contribution of the $\mathbf{p} \cdot \mathbf{A}$ term to scattering in addition to the \mathbf{A}^2 term, which alters the first term in (63) representing the scattering from the nuclear motion as follows:

$$I^{\text{nuc}}(q, \omega)/N \equiv \left| f_I(q) + \rho(q) - \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(\omega_0) - Z_B \right|^2 S_{II}(q, \omega). \quad (71)$$

Here, $\hat{\alpha}^{\text{ce}}(\omega_0)$ denotes the atomic polarizability defined by (51) (see appendix B). Thus, anomalous x-ray diffraction from the metallic system is described by the formula

$$I(q)/N \equiv \left| f_I(q) + \rho(q) - \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(\omega_0) - Z_B \right|^2 S_{II}(q) + Z_f S^0(q) + Z_B S_{\text{inc}}^I(q) \quad (72)$$

which reduces to the well known formula used to describe anomalous x-ray scattering [16] for non-metallic systems where $\rho(q) = 0$ and $Z_f = 0$. It is important to remember that the atomic polarizability $\hat{\alpha}^{\text{ce}}(\omega_0)$ in (72) should be determined for an ion in the presence of surrounding ions and electrons, instead of for an isolated ion as in the analysis of the anomalous x-ray diffraction experiment, and that we must take account of the presence of the Fermi surface of free electrons in the edge calculation, since an electron excited by a photon can be moved only to above the Fermi surface at zero temperature.

On the other hand, in the case of light (electromagnetic wave) scattering, equation (72) can be written as

$$I^{\text{nuc}}(q, \omega)/N = \left| Z_f - \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(0) \right|^2 S_{II}(q, \omega) \quad (73)$$

since in this case we can make the approximation $f_I(q) + \rho(q) - Z_B \simeq Z_f$, because of the wave-vector being nearly zero ($q \sim 0$). This expression reduces to the usual formula [28] for optical

Raman (inelastic Rayleigh) scattering for non-metallic fluids ($Z_f = 0$), which represents the Rayleigh line and the Brillouin lines as elastic and inelastic scattering, respectively [9].

In plasma physics, it is customary to call scattering from the free electrons Thomson scattering [29–34], which is described by the free-electron DSF:

$$S_{ee}(q, \omega) \equiv \frac{1}{2\pi Z_f N} \int_{-\infty}^{\infty} \langle \rho_f(q, t) \rho_f^*(q, 0) \rangle \exp(i\omega t) dt. \quad (74)$$

In plasma diagnostics by means of light scattering, Thomson scattering is considered to give the ion feature in addition to the electron feature, since the bunches of electrons which are a shield on each ion reflect the ion motion, and the free-electron DSF is divided into electron-feature and ion-feature parts: $S_{ee}(q, \omega) \equiv S_{ee}^e(q, \omega) + S_{ee}^i(q, \omega)$.

The free-electron DSF is determined from the fluctuation-dissipation theory as

$$S_{ee}(q, \omega) = - \int_{-\infty}^{\infty} \frac{\hbar \beta}{1 - \exp(-\beta \hbar \omega)} \frac{1}{\pi} \Im \chi_q^{\text{fe}}[\omega] d\omega \quad (75)$$

with the use of the free-electron density response function

$$\chi_q^{\text{fe}}[\omega] = \frac{\chi_q^{0e}[\omega]}{\epsilon_e(q, \omega)} + \frac{\rho(q, \omega)^2}{Z_f} \chi_q^{\text{II}}[\omega]. \quad (76)$$

Here,

$$\epsilon_e(q, \omega) \equiv 1 + n_0^e \beta v_{ee}(q) [1 - G(q, \omega)] \chi_q^{0e}[\omega] \quad (77)$$

$$\rho(q, \omega) \equiv n_0^e C_{el}(q, \omega) \chi_q^{0e}[\omega] / \epsilon_e(q, \omega). \quad (78)$$

In the above expressions, the free-electron density response function is exactly (but formally) represented using the dynamical electron–ion direct correlation function $C_{el}(q, \omega)$, and $\chi_q^{\text{II}}[\omega]$ is the ion–ion density response function [10]. Also, the electron cloud $\rho(q, \omega)$ surrounding each ion is approximated by a static one $\rho(q) \equiv \rho(q, 0)$ in the expression (76), since the electron motion is very rapid compared to the ion motion owing to the large mass difference between them. Then, there results from (75)

$$S_{ee}(q, \omega) = \frac{|\rho(q)|^2}{Z_f} S_{\text{II}}(q, \omega) + S_{ee}^0(q, \omega) \quad (79)$$

which provides the ion feature as the first term involving the ion–ion DSF $S_{\text{II}}(q, \omega)$ and the electron feature as the second term representing the ‘free’-electron DSF $S_{ee}^0(q, \omega)$ in (79), which was already shown as (38), to derive the absorption cross section in the previous section. It should be noted that this division of the free-electron density response function into ion and electron features in (76) is different from the usual division [29–31] used for Thomson scattering in plasma physics, and is more natural than that.

From a fundamental point of view, it is not correct to treat light scattering by plasmas only using the free-electron DSF $S_{ee}(q, \omega)$, since photons are scattered also by the core electrons coupled with the nuclear motion in a partially ionized plasma. By taking account of the core-electron contribution to light scattering, ‘Thomson’ scattering is described by

$$I^{\text{Thomson}}(q, \omega)/N \equiv \left| f_1(q) + \rho(q) - \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(0) - Z_B \right|^2 S_{\text{II}}(q, \omega) + Z_f S_{ee}^0(q, \omega) \quad (80)$$

and the third term $\tilde{S}^{\text{ce}}(q, \omega) \simeq \tilde{S}^{\text{ce}}(q, 0)$ of (63) yields the background scattering for this experiment. When the wavevector q is small and the atomic polarizability is negligible compared with Z_f , this expression reduces to

$$I^{\text{Thomson}}(q, \omega)/N \simeq Z_f^2 S_{\text{II}}(q, \omega) + Z_f S_{ee}^0(q, \omega) \quad (81)$$

which becomes identical with (79) due to $\rho(0) = Z_f$, and provides confirmation of the conventional experimental analysis for the small- q region. In this formula, the total scattering cross section is determined by

$$I^{\text{Thomson}}(q)/N = |f_1(q) + \rho(q) - \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(0) - Z_B|^2 S_{\text{II}}(q) + Z_f S_{\text{ee}}^0(q) \quad (82)$$

$$\simeq Z_f^2 S_{\text{II}}(q) + Z_f S_{\text{ee}}^0(q) \quad (83)$$

from which the ion-feature and electron-feature parts at zero wavevector are provided in the forms

$$I_{\text{ion}}^{\text{Thomson}}(0)/N = \left| Z_f - \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(0) \right|^2 n_0^I \kappa_T / \beta$$

(κ_T is the isothermal compressibility) and

$$I_{\text{ele}}^{\text{Thomson}}(0)/N = 0$$

respectively, while the large- q behaviours go like

$$\lim_{q \rightarrow \infty} I_{\text{ion}}^{\text{Thomson}}(q)/N = \left| Z_B + \frac{m}{e^2} \omega_0^2 \hat{\alpha}^{\text{ce}}(0) \right|^2$$

and

$$\lim_{q \rightarrow \infty} I_{\text{ele}}^{\text{Thomson}}(q)/N = Z_f.$$

These results show different behaviours from the ion and electron features of the usual definition, even in the weakly coupled classical-gas limit $n_0^I \kappa_T / \beta = 1/(Z_f + 1)$.

In addition to light scattering, it should be mentioned that inelastic x-ray scattering may be used for plasma diagnostics on the basis of (63); the electron feature $S_{\text{ee}}^0(q, \omega)$ may be easily observed. On the other hand, it will be difficult to measure the ion feature $S_{\text{II}}(q, \omega)$, observation of which requires a high-resolution experiment ($\Delta\omega \sim 10$ meV), although the ion–ion DSFs of liquid metals have been observed by Sinn *et al* [15] using inelastic x-ray scattering.

4. Conclusions

On the basis of the dipole approximation, we have derived the photoabsorption cross section (46) for a plasma or a liquid metal, which represents photoabsorption caused by the nuclear motion, the free-electron motion and the core-electron behaviour in the ion. Also, each term of (46) can be described, if necessary, in any form of the dipole–dipole correlation, the polarizability, the conductivity or oscillator strengths, as is given for the case of the core-electron photoabsorption in (55a)–(55d). It should be noticed that some part $\rho(q)$ of the free electrons contributes to the photoabsorption due to the nuclear motion as the screening charge, while the other part constitutes the so-called free–free absorption; this absorption does not come from the atomic polarization $\hat{\alpha}^{\text{ce}}(\omega)$ of (55a) as was frequently recognized in the form $\hat{\alpha}_{\text{ff}}^{\text{ce}}(\omega)$.

On the other hand, the standard method of calculating the electron Bremsstrahlung in a plasma is based on a model where a photon is radiated or absorbed in the scattering of an electron by an *isolated* atom or ion [35]: this model may be described by (2). However, as the density of a plasma is increased and the coupling of particles in a plasma becomes strong, the isolated-atom model and the term $\mu_q^{\text{fe}}(\omega)$ in (46) will be shown to give different results from each other to a large extent. In contrast to the case of the free–free absorption, the bound–bound and bound–free absorptions can be obtained by treating a *single* ion in a plasma, as the

third term of (46) indicates. The absorption cross section $\sigma_a^{ce}(\omega)$ due to the core electron in a plasma can be determined from the density–density response function for a single ion by (51), which can be evaluated by the Zangwill method [36] with its extension to take account of the surrounding ions and electrons in the presence of the Fermi surface. This approach based on (46) will produce a significantly different result from that for an isolated atom as usually used for the plasma spectroscopy. This programme is now in progress.

The absorption cross section in the dipole approximation is related to the photon scattering cross section as the relation (16) indicates. In the derivation of the absorption cross section, the form factor approximation (23) plays an important role for deriving the expression for the total DSF. It is important to remember that this approximation is well established for x-ray diffraction experiments. Also, the ‘metallic’ form factor $f_I(q) + \rho(q)$ should be thought of as an established approximation, since the x-ray diffraction of all liquid metals is analysed with the use of the atomic form factor $f_A(q)$, which is almost identical to the metallic form factor $f_I(q) + \rho(q)$. This experimental fact lends support to the photoabsorption expression (46) through the relation (16).

On the other hand, the photon scattering formulae, (63) and (71), provide a wide view of photon scattering experiments; we can see the whole mechanism of photon scattering in a single formula, which can be used to observe any motion in the system containing the nuclear motion the free-electron motion or the core-electron behaviour of the ion. Since the structure of the background scattering for each experiment is clearly defined, a combination of several kinds of experiment provides reliable data.

In usual analysis of the anomalous x-ray scattering experiment, the anomalous scattering factor $(m/e^2)\omega_0^2\hat{\alpha}^{ce}(\omega_0) + Z_B$ is taken from the result calculated for a neutral atom, even in a metal. It should be noted that the anomalous form factor for the metallic system is different from that for the non-metallic system; $f_A(q)$ is replaced by $f_I(q) + \rho(q)$ and the atomic polarizability $\hat{\alpha}^{ce}(\omega_0)$ should be calculated for a metallic state taking account of the effects of the surrounding ions and electrons in addition to the presence of the Fermi surface.

The so-called Thomson scattering in plasma physics is nothing but ‘light’ scattering from a plasma; a light scattering formula (71) for a plasma derived in the present work has proved that ‘Thomson’ scattering is described only by the free-electron DSF for the small- q region. Also, we proposed a more natural division of Thomson scattering into the ion feature and the electron feature, as given by (79).

The most fundamental assumption made in deriving the photoabsorption and scattering formulae is that a liquid metal or a plasma can be considered as an electron–ion mixture. For a liquid metal, there is no problem in using this model, especially for a simple metal. On the other hand, for a plasma, the ion in this theory is only the average ion; there are many kinds of charge state in general. Therefore, in order to compare the result of this model with experiments, we need further refinement, such as a combined use of the Saha equation to determine the charge population [37]: this problem remains for future work.

Appendix A

The photoabsorption cross section owing to the core electrons in the ion can be represented by the core-electron DSF as

$$\mu_q^{ce}(\omega) \equiv \frac{1}{Z_B} \int_{-\infty}^{\infty} \langle j_q^{ce*}(0) \cdot j_q^{ce}(t) \rangle_L e^{-i\omega t} dt \quad (A.1)$$

$$= 2\pi \frac{\omega^2}{q^2} S_{ee}^{ce}(q, \omega) = 2\pi \frac{\omega^2}{q^2} \tilde{S}_{ee}^{ce}(q, \omega) \quad (A.2)$$

where equation (A.2) results from the fact that $S_{\text{ee}}^{\text{ce}}(q, \omega)$ differs from $\tilde{S}_{\text{ee}}^{\text{ce}}(q, \omega)$ only by the term $\delta(\omega)$, as defined in (35). Therefore, the zero- q limit of the core-electron DSF divided by q^2 :

$$\frac{\tilde{S}^{\text{ce}}(q, \omega)}{q^2} \equiv \frac{1}{2\pi Z_{\text{B}}} \int_{-\infty}^{\infty} \frac{\tilde{I}^{\text{ce}}(q, t)}{q^2} e^{-i\omega t} dt \quad (\text{A.3})$$

can be calculated by taking this limit:

$$\lim_{q \rightarrow 0} \frac{\tilde{I}^{\text{ce}}(q, t)}{q^2} \equiv \lim_{q \rightarrow 0} \frac{1}{q^2} \int \int d\mathbf{r} d\mathbf{r}' e^{-iq \cdot \mathbf{r}} \langle \delta \rho_{\text{B}}(\mathbf{r}, 0) \delta \rho_{\text{B}}(\mathbf{r}', t) \rangle e^{iq \cdot \mathbf{r}'} \quad (\text{A.4})$$

$$= \int \int d\mathbf{r} d\mathbf{r}' z \langle \delta \rho_{\text{B}}(\mathbf{r}, 0) \delta \rho_{\text{B}}(\mathbf{r}', t) \rangle z' \quad (\text{A.5})$$

$$= \langle z(0)z(t) \rangle = \frac{1}{3} \langle \mathbf{r}(0) \cdot \mathbf{r}(t) \rangle \quad (\text{A.6})$$

which gives rise to the dipole–dipole correlation

$$\lim_{q \rightarrow 0} \frac{e^2 \tilde{S}^{\text{ce}}(q, \omega)}{q^2} = \frac{1}{2\pi Z_{\text{B}}} \int_{-\infty}^{\infty} \frac{1}{3} \langle \mathbf{d}(0) \cdot \mathbf{d}(t) \rangle e^{-i\omega t} dt \quad (\text{A.7})$$

with

$$\mathbf{d}(t) = e\mathbf{r}(t) \equiv e\mathbf{r} \sum_{i \in \text{bound}} \delta(\mathbf{r} - \mathbf{r}_i(t)). \quad (\text{A.8})$$

In a similar way, we can obtain the atomic polarizability by taking this limit:

$$\lim_{q \rightarrow 0} \frac{e^2 \chi_q^{\text{ce}}[\omega]}{q^2} \equiv \lim_{q \rightarrow 0} \frac{e^2}{q^2} \int \int d\mathbf{r} d\mathbf{r}' e^{-iq \cdot \mathbf{r}} \chi^{\text{ce}}(\mathbf{r}, \mathbf{r}'; \omega) e^{iq \cdot \mathbf{r}'} \quad (\text{A.9})$$

$$= \frac{e^2}{3} \int \int d\mathbf{r} d\mathbf{r}' (\mathbf{r} \cdot \mathbf{r}') \chi^{\text{ce}}(\mathbf{r}, \mathbf{r}'; \omega) \quad (\text{A.10})$$

$$\equiv -\hat{\alpha}^{\text{ce}}(\omega). \quad (\text{A.11})$$

Here, the density–density response function $\chi_q^{\text{ce}}[\omega]$ is defined explicitly by

$$\chi_q^{\text{ce}}[\omega] \equiv \frac{1}{Z_{\text{B}}} \int_0^{\infty} e^{i\omega t} \left\langle \frac{1}{i\hbar} [\rho_{\text{B}}(\mathbf{q}, t), \rho_{\text{B}}^*(\mathbf{q}, 0)] \right\rangle dt \quad (\text{A.12})$$

$$= \frac{1}{Z_{\text{B}}} \sum_{\text{ba}} p_{\text{a}} |\langle \text{b} | \rho_{\text{B}}^*(\mathbf{q}) | \text{a} \rangle|^2 \left\{ \frac{1}{\omega - \omega_{\text{ba}} + i\eta} - \frac{1}{\omega + \omega_{\text{ba}} + i\eta} \right\} \quad (\text{A.13})$$

with $\hbar\omega_{\text{ba}} \equiv E_{\text{b}} - E_{\text{a}}$.

On the other hand, equation (54) results from the relation between the conductivity and the polarizability:

$$\hat{\sigma}_{\text{L}}(\omega) = -i\omega \hat{\alpha}(\omega) \quad (\text{A.14})$$

which is the zero- q limit of the general relation between the longitudinal conductivity and the density response function [8]:

$$\hat{\sigma}_{\text{L}}[q, \omega] \equiv \frac{e^2}{N} \int_0^{\infty} \beta \langle \mathbf{j}_{\text{q}}^*(0); \mathbf{j}_{\text{q}}(t) \rangle_{\text{L}} e^{i\omega t} dt = i\omega \frac{e^2 \chi_q[\omega]}{q^2}. \quad (\text{A.15})$$

The absorption coefficient $k(\omega)$ [38] is defined in the form

$$k(\omega) \equiv \frac{2\omega \Im \hat{n}}{c} = \frac{2\omega \Im \hat{\epsilon}^{1/2}}{c} \quad (\text{A.16})$$

by using the complex refractive index \hat{n} , which is given by the dielectric constant $\hat{\epsilon}$:

$$\hat{\epsilon}(\omega) \equiv 1 + \frac{4\pi\sigma_L}{\omega}i = 1 + 4\pi n_I \hat{\alpha}(\omega). \quad (\text{A.17})$$

This definition of $k(\omega)$ provides an approximate expression for the case where $\hat{\epsilon}'' \ll \hat{\epsilon}'$:

$$k(\omega) \approx \frac{\omega \hat{\epsilon}''(\omega)}{n(\omega)c} = \frac{4\pi \Re \sigma_L(\omega)}{n(\omega)c} = \frac{4\pi \omega n_I \Im \hat{\alpha}(\omega)}{n(\omega)c} \quad (\text{A.18})$$

with the refractive index $n(\omega) \approx \sqrt{\Re \hat{\epsilon}(\omega)}$.

Appendix B

Interaction of electrons with the radiation field $\mathbf{A}(\mathbf{r})$ is described by the Hamiltonian

$$H_1 = H_1 + H_2 \quad (\text{B.1})$$

consisting of two terms: the $\mathbf{p} \cdot \mathbf{A}$ term,

$$H_1 = -\frac{e^2}{2mc^2} \sum_i \mathbf{p}_i \cdot \mathbf{A}(\mathbf{r}_i) \Rightarrow -\frac{e}{mc} \sum_q \left(\frac{2\pi\hbar c^2}{V\omega_q} \right)^{1/2} \{P(\mathbf{q})a_q + P^\dagger(\mathbf{q})a_q^\dagger\} \quad (\text{B.2})$$

which is in the second-quantized representation used to describe the photon absorption, and the \mathbf{A}^2 term,

$$H_2 \equiv \frac{e^2}{2mc^2} \sum_i A_i^2 \quad (\text{B.3})$$

$$\Rightarrow \frac{e^2}{2mc^2} \sum_{kk'} \left(\frac{2\pi\hbar c^2}{V\sqrt{\omega_k\omega_{k'}}} \right) (\mathbf{e}_k \cdot \mathbf{e}_{k'}) \left[\sum_j e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_j} \right] [a_k a_{k'}^\dagger + a_{k'}^\dagger a_k] \quad (\text{B.4})$$

which generates the photon scattering, with

$$P(\mathbf{k}) \equiv \sum_j (\mathbf{e}_k \cdot \mathbf{p}_j) \exp[i\mathbf{k} \cdot \mathbf{r}_j]. \quad (\text{B.5})$$

Since any bound electron j can be thought to belong to some ion α in the system, we can represent its coordinate as $\mathbf{r}_j = \mathbf{R}_\alpha + \mathbf{r}_{j\alpha}$; therefore, we can obtain an approximate expression for (B.5) in the form

$$P(\mathbf{k}) \approx \sum_\alpha \exp[i\mathbf{k} \cdot \mathbf{R}_\alpha] P^\alpha(\mathbf{k}) \quad (\text{B.6})$$

with

$$P^\alpha(\mathbf{k}) \equiv \sum_j (\mathbf{e}_k \cdot \mathbf{p}_{j\alpha}) \exp[i\mathbf{k} \cdot \mathbf{r}_{j\alpha}] \equiv P^0(\mathbf{k}). \quad (\text{B.7})$$

As a result of (B.6), we can define the transition matrix of each ion α going from an initial state $I = \omega_0, \mathbf{k}_0, \mathbf{e}_0$ to a final state $F = \omega_1, \mathbf{k}_1, \mathbf{e}_1$ by

$$\begin{aligned} F_{FI}^\alpha(\omega_0, \omega_1) &\equiv \langle F_e | H_2^\alpha | I_e \rangle + \sum_N \frac{\langle F_e | H_1^\alpha | N \rangle \langle N | H_1^\alpha | I_e \rangle}{E_I - E_N} \\ &= e^{i(\mathbf{k}_0 - \mathbf{k}_1) \cdot \mathbf{R}_\alpha} \left\{ \langle F_e | \sum_i \exp[i(\mathbf{k}_0 - \mathbf{k}_1) \cdot \mathbf{r}_{i0}] | I_e \rangle (\mathbf{e}_0 \cdot \mathbf{e}_1) \right. \\ &\quad \left. + \sum_N \frac{\langle F_e | H_1^{\text{ce}} | N \rangle \langle N | H_1^{\text{ce}} | I_e \rangle}{E_I - E_N} \right\}. \end{aligned} \quad (\text{B.8})$$

Therefore, the transition matrix for all ions in the system is written as

$$\begin{aligned}
 F_{FI}(\omega_0, \omega_1; \{R_\alpha\}) &\equiv \sum_\alpha F_{FI}^\alpha(\omega_0, \omega_1) \\
 &= \left[\sum_\alpha e^{i(k_0 - k_1) \cdot R_\alpha} \right] \left\{ \langle F_e | \sum_i \exp[i(k_0 - k_1) \cdot r_{i0}] | I_e \rangle (e_0 \cdot e_1) \right. \\
 &\quad - \frac{1}{m} \sum_N \left[\frac{\langle F_e | P^0(\mathbf{k}_0) | N \rangle \langle N | P^{0\dagger}(\mathbf{k}_1) | I_e \rangle}{\epsilon_N - \epsilon_I + \hbar\omega_1} \right. \\
 &\quad \left. \left. + \frac{\langle F_e | P^{0\dagger}(\mathbf{k}_1) | N \rangle \langle N | P^0(\mathbf{k}_0) | I_e \rangle}{\epsilon_N - i\eta - \epsilon_I - \hbar\omega_0} \right] \right\}. \tag{B.9}
 \end{aligned}$$

Now, the second term in the large bracket can be written in the elastic approximation [39] in the form

$$\begin{aligned}
 \frac{1}{m} \sum_N \left[\frac{\langle I_e | P^{0\dagger}(\mathbf{k}_0) | N \rangle \langle N | P^0(\mathbf{k}_0) | I_e \rangle}{\hbar\omega_0 - \hbar\omega_{N0} + i\eta} - \frac{\langle I_e | P^0(\mathbf{k}_0) | N \rangle \langle N | P^{0\dagger}(\mathbf{k}_0) | I_e \rangle}{\hbar\omega_0 + \hbar\omega_{N0}} \right] \\
 = e_1 \cdot m \chi_{JJ}^{\text{ce}}(-\mathbf{k}_0, \omega_0) \cdot e_0 \tag{B.10}
 \end{aligned}$$

$$= e_1 \cdot m \chi_{JJ}^{\text{ce}}(\mathbf{k}_0, \omega_0) \cdot e_0 \tag{B.11}$$

in terms of the current–current correlation function $\chi_{JJ}^{\text{ce}}(\mathbf{k}_0, \omega_0)$ [40] for the core electrons in each ion ($\hbar\omega_{N0} \equiv \epsilon_N - \epsilon_I$). Because of the relation [40]

$$\lim_{k \rightarrow 0} m \chi_{JJ}^{\text{ce}}(\mathbf{k}, \omega) = \left[\lim_{k \rightarrow 0} m \frac{\omega^2}{k^2} \chi_k^{\text{ce}}[\omega] - Z_B \right] \mathbf{1} = \left[-\frac{m}{e^2} \omega^2 \hat{\alpha}^{\text{ce}}(\omega) - Z_B \right] \mathbf{1} \tag{B.12}$$

which shows that the current–current correlation in the zero-wavevector limit can be represented by the atomic polarizability, the transition matrix (B.9) in the dipole approximation (B.12) can be written finally in the form

$$F(\omega_0; \{R_\alpha\}) = [f_I(q) - m\omega_0^2 \hat{\alpha}^{\text{ce}}(\omega_0)/e^2 - Z_B] \left[\sum_\alpha e^{i\mathbf{q} \cdot R_\alpha(t)} \right] (e_0 \cdot e_1) \tag{B.13}$$

$$\equiv F_{\text{ion}}(q, \omega_0) \rho_I(q, t) (e_0 \cdot e_1) \tag{B.14}$$

with $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_1$. This indicates that, for the resonant case, the approximation $\rho_c(q, t) = f_I(q) \rho_I(q, t)$ of (23) should be replaced by $\rho_c(q, t) = F_{\text{ion}}(q, \omega_0) \rho_I(q, t)$, which leads to the expression for anomalous scattering (71).

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