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X-ray Thomson scattering in warm dense matter

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Abstract. The scattering of photons in plasmas is an important diagnostic tool. Especially, the region of warm dense matter can be probed by X-ray Thomson scattering. The scattering cross-section is related to the dynamic structure factor $S(k, \omega)$. We improve the standard treatment of the scattering on free electrons within the random phase approximation (RPA) by including collisions. The dielectric function is calculated in the Born–Mermin approximation. The inclusion of collisions modifies the dynamic structure factor significantly in the warm dense matter regime. We conclude that a theoretical description beyond the RPA is needed to derive reliable results for plasma parameters from X-ray Thomson scattering experiments.

PACS. 52.25.Os Emission, absorption, and scattering of electromagnetic radiation – 52.70.La X-ray and gamma-ray measurements – 61.10.Eq X-ray scattering (including small-angle scattering) – 71.10.Ca Electron gas, Fermi gas

Rapid Note

1 Introduction

Thomson scattering in plasmas has been studied for a long time [1–5]. Its cross-section is directly related to the dynamic structure factor $S(k, \omega)$. Therefore, Thomson scattering can serve as a perfect tool to either analyze the plasma parameters, or to test the quality of the model used to determine the dynamic structure factor.

The study of dense plasmas is relevant for, e.g., inertial confinement fusion experiments or models for stellar interiors and requires appropriate diagnostic methods. Dense plasmas are opaque in the optical region so that X-rays instead of optical lasers have to be used to probe the plasma. In particular, solid density plasmas at low temperatures of several eV as occurring in planetary interiors are of special interest. Strong coupling effects are important under those conditions which are also characterized as warm dense matter states.

Powerful X-ray sources are needed for this purpose. High-power optical lasers can produce intense X-ray pulses to pump and probe samples at solid densities [6–9]. Alternatively, a free electron laser (FEL) test facility at DESY Hamburg has already demonstrated its great capacities for high-flux and time-resolved experiments at about 100 nm wavelength [10]. The building of an X-ray FEL is planned at DESY in Hamburg [11], and a FEL facility operating in the VUV range from 60-5 nm will start by end of 2004. A similar project is installed at SLAC in Stanford [12].

On the other hand, a consistent many-body theory is needed for the evaluation of the Thomson scattering signal from dense plasmas in order to derive plasma parameters such as the electron temperature and density as well as the ionization state. For instance, one has to treat the X-ray scattering from electrons bound to the nuclei as well as from free electrons as described recently in detail by Gregori et al. [13]. Furthermore, strong correlations and scattering processes between the plasma constituents (electrons, ions) may become of importance.

First measurements of the averaged ionization state $\bar{Z}$, the electron density, and the electron temperature by using incoherent Thomson scattering at a probe wavelength of $\lambda = 263\,\text{nm}$ were performed for high-Z (Au) plasmas [14,15]. Spectrally resolved X-ray Thomson scattering at $\lambda = 0.24$ nm was applied to determine plasma parameters for dense Be plasma [7]; results for Be at solid densities were given recently [9]. Comparison of the experimentally determined ionization state with the ACTEX model [16] and generalized Saha equations including nonideality corrections [17] shows good agreement. Similar measurements were performed for carbon plasma at solid densities [18].

So far, within the context of Thomson scattering, analytic results for the dynamic structure factor were presented on the level of the random phase approximation (RPA), see [13]. Strong coupling effects were analysed recently within the scheme of local field corrections using an interpolation of its low- and high-frequency limits [19].

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Collisional broadening effects on ion-acoustic modes were treated using a modified Mermin formalism [20].

Here we demonstrate that it is necessary to go beyond the RPA by including collisions in order to obtain reliable results for plasma parameters in the warm dense matter region using Thomson scattering. The dynamic collision frequency $\nu(\omega)$ is calculated in Born approximation within linear response theory [21,22]. The k-dependent dielectric function is obtained via a generalized Mermin formula [23,24]. We show that these improvements have a significant influence on the dynamic structure factor in the warm dense matter regime and, thus, also on the interpretation of the Thomson scattering signal.

2 Dynamic structure factor: Born–Mermin approximation

In this paper, we use the terminology as found in [2,5,13]. In particular, the differential scattering cross-section is related to the total dynamic structure factor $S(k,\omega)$ of all electrons in the plasma according to

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \sigma_{\rm T}\frac{k_1}{k_0} S(k,\omega), \quad (1)$$

where $\sigma_{\rm T}$ is the Thomson cross-section [5]; k_0 and k_1 are the wavenumbers of the incident and the scattered light. The energy and momentum transfer is characterized by $\hbar\omega = \hbar\omega_0 - \hbar\omega_1$ and $\hbar\mathbf{k} = \hbar\mathbf{k}_0 - \hbar\mathbf{k}_1$, respectively. As outlined in [5], the structure factor contains contributions from free electrons, electrons tight to the ion motion including screening, and of inelastic scattering off core electrons. We will focus on the free electron part of the dynamic structure factor in this work without further specifying the ionic system.

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The dynamic structure factor $S(k,\omega)$ and the longitudinal dielectric function $\epsilon(k,\omega)$ are related via the fluctuation-dissipation theorem:

$$S(k,\omega) = -\frac{\epsilon_0\hbar k^2}{\pi e^2 n_{\rm e}}\frac{{\rm Im}\,\epsilon^{-1}(k,\omega)}{1-\exp\left(-\hbar\omega/k_{\rm B}T_{\rm e}\right)}. \quad (2)$$

In RPA, the dielectric function reads

$$\epsilon^{\rm RPA}(k,\omega) = 1 - \frac{e^2}{\epsilon_0 k^2 \Omega_0}\sum_p \frac{f_{p+k/2} - f_{p-k/2}}{\Delta E_{p,k} - \hbar(\omega + i\eta)}, \quad (3)$$

with $\Delta E_{p,k} = E_{p+k/2} - E_{p-k/2} = \hbar^2\mathbf{k}\cdot\mathbf{p}/m_{\rm e}$. Here, $f_p = \{\exp[(E_p-\mu)/(k_B T)]+1\}^{-1}$ denotes the Fermi distribution function with μ the chemical potential of the free electrons.

Improvements of the RPA dielectric function can be derived from the Mermin formula [23]. Utilizing consistent linear response theory [24], a dynamic collision frequency $\nu(\omega)$ occurs instead of a static relaxation time in the Mermin dielectric function $\epsilon^{\rm M}(k,\omega)$:

$$\epsilon^{\rm M}(k,\omega) - 1 = \frac{\left(1 + i\frac{\nu(\omega)}{\omega}\right)\left[\epsilon^{\rm RPA}(k,\omega + i\nu(\omega)) - 1\right]}{1 + i\frac{\nu(\omega)}{\omega}\frac{\epsilon^{\rm RPA}(k,\omega+i\nu(\omega))-1}{\epsilon^{\rm RPA}(k,0)-1}}. \quad (4)$$

The complex valued dynamic collision frequency is related to the dynamic conductivity $\sigma(\omega)$ in the long wavelength limit via a generalized Drude expression [21,25]

$$\sigma(\omega) = i\epsilon_0\omega[\epsilon(0,\omega) - 1] = \frac{\epsilon_0\,\omega_{\rm pe}^2}{-i\omega + \nu(\omega)}, \quad (5)$$

with the electronic plasma frequency $\omega_{\rm pe}^2 = n_{\rm e}e^2/(\epsilon_0 m_{\rm e})$. Within the Zubarev approach of linear response theory, the dynamic collision frequency is expressed by a force-force correlation function which can be evaluated in different approximations [26]. In Born approximation with respect to the statically screened Coulomb potential,

$$V_{\rm D}(k) = \frac{e^2}{\epsilon_0\Omega_0}\frac{1}{(k^2 + 1/\lambda_{\rm D}^2)}, \quad \lambda_{\rm D}^2 = \frac{\epsilon_0 k_B T_{\rm e}}{n_{\rm e}e^2}, \quad (6)$$

the following result is obtained [21]:

$$\nu_{\rm dyn}^{\rm Born}(\omega) = -ig\,n_{\rm e}\int_0^\infty dy\,\frac{y^4}{(\bar{n}+y^2)^2} \times \int_{-\infty}^{\infty} dx\,{\rm e}^{-(x-y)^2}\frac{1-{\rm e}^{-4xy}}{xy(xy - \bar{\omega} - i\eta)}. \quad (7)$$

The prefactor g is given by

$$g = \frac{e^4\beta^{3/2}}{24\sqrt{2}\pi^{5/2}\epsilon_0^2 m_{\rm e}^{1/2}}, \quad (8)$$

and the other quantities are defined by $\bar{\omega} = \hbar\omega/(4k_B T)$ and $\bar{n} = \hbar^2/(8m_{\rm e}\lambda_{\rm D}^2 k_B T)$. The present combination of the Mermin dielectric function (4) including collisions in dynamic Born approximation (7) is defined as Born–Mermin approximation (BMA) in what follows.

3 Numerical evaluation and plasma diagnostic

In order to allow direct comparison with [13], we consider the same plasma conditions as summarized in Table 1 by the sets $\mathbf{a}i$, $\mathbf{b}i$, and $\mathbf{c}i$ with $i = 1, 2, 3$.

Plasmas characterized by the parameter set $\mathbf{a}i$ are accessible with optical lasers, while light in the extreme ultraviolet (EUV) range has to be used for the conditions of set $\mathbf{b}i$. Plasmas with parameters given by set $\mathbf{c}i$ can be diagnosed with X-rays. In the last column of Table 1, the results for the static collision frequency in Born approximation are given. For the parameter set $\mathbf{a}i$, collisions are much less important than in the case of higher densities.

Table 1. Plasma parameters as considered in [13]: electron density n_e, the corresponding electron plasma frequency ω_{pe}, initial laser wavelength λ_0, scattering angle θ_{sc}, electron temperature T_e, and static collision frequency in Born approximation.

	n_e (cm^{-3})	ω_{pe} (eV)	λ_0 (nm)	θ_{sc}	T_e (eV)	$\mathrm{Re}\,\nu_{stat}^{Born}$ (ω_{pe})
a1					200	0.00044
a2	10^{19}	0.117	532	90°	600	0.00010
a3					3000	0.00001
b1					0.5	0.6538
b2	10^{21}	1.174	4.13	160°	2.0	0.5305
b3					8.0	0.1574
c1					0.8	0.0137
c2	10^{23}	11.742	0.26	60°	3.0	0.1393
c3					13.0	0.2090

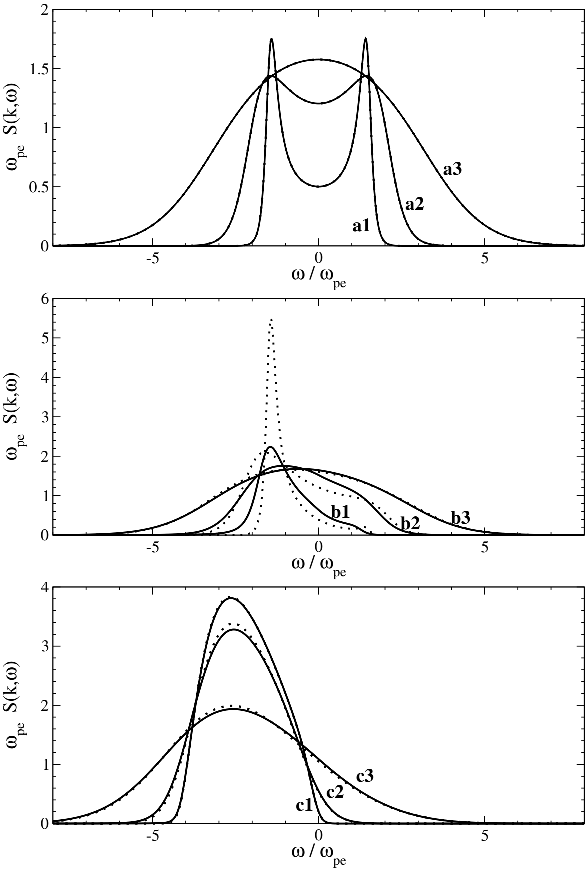

Fig. 1. $S(k,\omega)$ for plasmas with parameters according to Table 1. Full lines: collisions included via the BMA; dotted lines: RPA (collisions neglected).

In Figure 1, the free electron dynamic structure factor is shown for the corresponding parameters of Table 1. The RPA results, as already presented in [13], are compared with the BMA.

The influence of collisions is most important in the EUV domain at densities of about $n_e = 10^{21}$ cm^{-3}, i.e. for the parameter set **b***i*. Collisions broaden the structure factor and shift the position of the peak to higher energies. For the low-density case **a***i*, the RPA is applicable and collisions don't play any role as expected. In the high-density case **c***i*, where ν/ω_{pe} is comparable to the case **b***i*, Pauli blocking prevents a major influence of collisions on the dynamic structure factor.

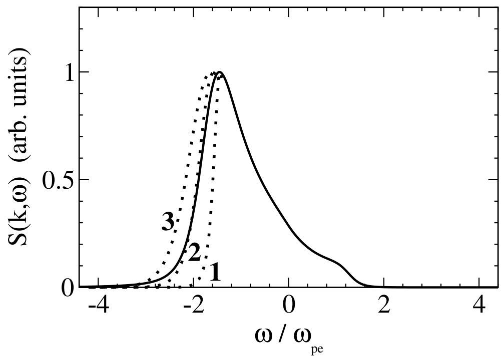

Fig. 2. Comparison of $S(k,\omega)$ calculated within the BMA for the parameter set **b**1, i.e. $T_e = 0.5$ eV (full line), with RPA results for different electron temperatures T_e^{RPA} (dotted lines; **1**: 0.5 eV, **2**: 1.0 eV, **3**: 1.5 eV).

In Figure 2, we show that the electron temperature derived from the dynamic structure factor can change significantly if collisions in the plasma are taken into account. We compare the high-frequency wing of the dynamic structure factor calculated within the BMA for parameter set **b**1, i.e. $T_e = 0.5$ eV, with the corresponding RPA results for different temperatures.

A good agreement is found if a temperature of $T_e^{RPA} = 1.0$ eV is assumed. Thus, for these plasma parameters, a temperature inferred from the RPA structure factor overestimates that given by the dynamic Born result by a factor of two. This is of fundamental importance for the diagnostics of dense plasmas. Furthermore, results for quantities such as the ionization state will strongly be affected if models are used for which the plasma temperature is an input, see [17].

4 Conclusions

Our results for the free electron dynamic structure factor show that collisions become important in a region with a degeneracy parameter $\Theta \approx 1$ and coupling parameters $\Gamma \geq 1$. In particular, this applies to conditions relevant for the next stage of the free electron laser at DESY. Therefore, the use of Thomson scattering as a diagnostic tool for warm and dense matter requires to go beyond the standard RPA description and to account for a dynamic collision frequency as has been shown here.

Improved approximations for the collision frequency beyond the Born approximation are, in principle, needed (i) to indicate the range where collisions are important for the determination of plasma parameters, and (ii) to improve the accuracy of thermodynamic data inferred from Thomson scattering experiments. Results for a dynamic collision frequency accounting for dynamic screening as well as strong collisions can be gained from an ansatz proposed by Gould and DeWitt [27]:

$$\nu^{\mathrm{GD}}(\omega) = \nu^{\mathrm{ladder}}(\omega) - \nu^{\mathrm{Born}}(\omega) + \nu^{\mathrm{LB}}(\omega). \quad (9)$$

Dynamic screening is considered by the solution of a Lenard–Balescu (ν^{LB}) equation, whereas strong collisions are treated by a ladder approximation with respect to a statically screened potential (ν^{ladder}). Furthermore, the influence of higher moments on the collision frequency can be treated by a renormalization factor [21,28].

The connection of our approach to the concept of dynamic local field corrections (DLFC) to the RPA was outlined in reference [21]. Evaluations of DLFC by using a static collision frequency were performed for solid density LiH plasma [19], i.e. case **c***i*, and show also only marginal effects on the structure factor for conditions as considered here. Significant modifications of the RPA spectrum are found, however, for certain scattering angles where collective scattering is probed. For a complete description of Thomson scattering, ions and bound states have to be considered as well. These topics are subject of future studies on Thomson scattering in dense plasmas.

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