Ion Structure for X-Ray Thomson Scattering in Dense Fusion Plasmas

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Abstract.   The properties of the ion feature of the Thomson scattering signal are investigated. Firstly, the description of the atomic form factor by hydrogen-like wave functions is reviewed and better screening charges are obtained. Then the ionic structure in systems with several ion species is calculated from the HNC integral equation.

1. Introduction

X-ray Thomson scattering is one of the few potential diagnostic methods applicable for dense plasmas as they occur in all inertial fusion scenarios. The method is well-tested to yield detailed information for the plasma properties. Recent experiments with X-rays have demonstrated its capability to obtain the density, ionization degree and collision rate in solid-density plasmas [1, 2, 3]. Neglecting the very small contribution directly scattered from the ions, the intensity of the scattered light is determined by the differential scattering cross section

$$\frac{d^2\sigma}{d\Omega d\omega} = \sigma_T \frac{k_1}{k_0} S_{ee}^{tot}(k,\omega) \ , \tag{1}$$

where σ_T is the total Thomson cross section, k and ω denote the shifts in wave number and frequency, respectively, that the X-ray photons experience. $S_{ee}(k,\omega)$ is the dynamic electron structure factor. Even for weakly coupled plasmas, that is within the random phase approximation, the electron structure factor includes properties of the ionic subsystem [4]. For strongly coupled and partially ionized plasmas, it is given by [5, 6]

$$S_{ee}^{tot}(k,\omega) = |f_i(k) + q(k)|^2 S_{ii}(k,\omega) + Z_f S_{ee}^0(k,\omega) + Z_c \int \tilde{S}_{ce}(k,\omega - \omega') \, S_s(k,\omega) \, d\omega \ . \tag{2}$$

The first term considers the electrons co-moving with the ions: $f_i(k)$ is the atomic form factor describing the elastic scattering from bound electrons, $q(k)$ contains the contribution from the electrons in the screening cloud around the ion. The small frequency scale defined by the ion-ion structure factor $S_{ii}(k,\omega)$ cannot currently be resolved experimentally. It is therefore sufficient to describe the ion structure with the static structure factor $S_{ii}(k)$. The second term in Eq. (2) describes the scattering due to free electrons which can be spectrally resolved in the experiments [3]. The third term describes inelastic excitations within an atom or ion. It can usually be neglected in low-Z materials as the probed beryllium plasmas.
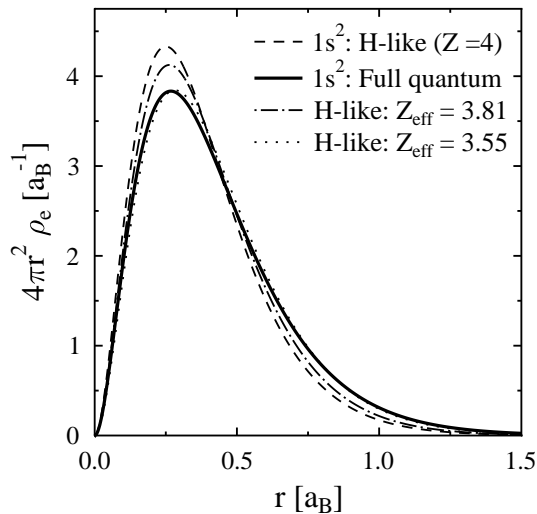
Figure 1. Comparison for the bound electron density around a doubly ionized beryllium ion. For the hydrogen-like model, the core charge is used as a fit parameter to yield agreement with numerical solutions.
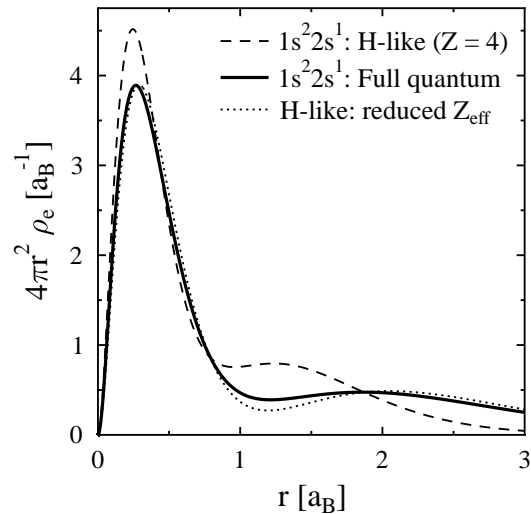
Figure 2. As for Fig. 1, but for a singly ionized beryllium ion. The effective charge states of the core that best fit the numerical data are $Z_{\mathrm{eff}} = 3.48$ for the 1s states and $Z_{\mathrm{eff}} = 2.55$ (2s state).

Although the ion structure results in a well-pronounced peak for low frequency shifts, this information cannot be used to infer the ion properties yet. The missing link is a reliable theoretical description of the ion structure and the nonlinear response of the electrons to the ions. Here, we calculate the ion properties using integral equations known from fluid theory [7]. In contrast to the often applied Yukawa model or two component calculations [8, 9], the numerical procedure used is not limited with respect to the number of species treated. In this contribution, we use this ability to focus on systems with multiple ion species. They always occur in systems with different chemical elements as plastics and also in plasmas with multiple ionization stages. Furthermore, we review the calculation of the atomic form factor using hydrogen-like wave functions.

2. Atomic Form Factor for Light Elements

One of the input quantities for the total electron structure factor (2) and therefore for the analysis of the Thomson scattering signal is the atomic form factor $f_i(k)$. For light elements as considered in the experiments, such as beryllium, only 1s and 2s electrons occur. The idea for a fast analysis code is to describe these bound states by hydrogen-like wave functions. However, one has to consider partial screening of the ionic core if more than one bound electron remains with the ion. This effects is usually described by an effective core charge.

Present models for the atomic form factor use fits to Hartree-Fock calculations [2]. Here, we use a different approach by employing solutions of a full (anti-symmetrized) Schrödinger equation. As before, we then use the effective core charge as a fit parameter to yield hydrogenic wave functions that reproduce the numerical results.

Fig. 1 shows a comparison of different calculations for a doubly charged beryllium ion. Clearly, just adding two hydrogen wave functions for the full charge of the nucleus does not yield agreement with the solution from the Schrödinger equation (thick full line). Even the screening charge of $Z_{\mathrm{scr}} = 0.19$, which reproduces the Hartree-Fock calculations and is used in present models [2], cannot sufficiently describe the exact solution. We have to increase the
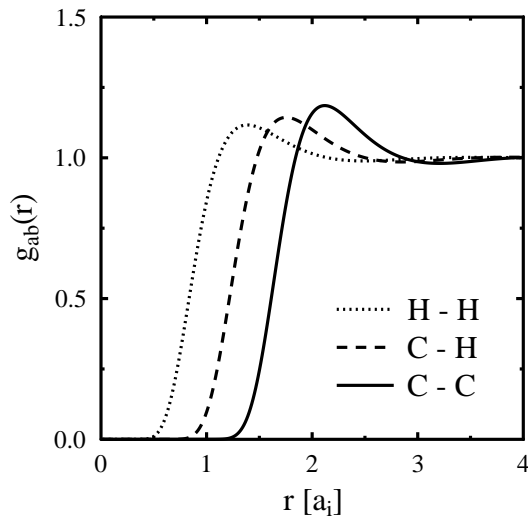
Figure 3. Pair distribution functions for the ions in a CH_4 plasmas with fully ionized hydrogen ions and four-fold ionized carbon. The plasma temperature is $T = 2.5 \times 10^4$ K and the ion densities are $n_C = 10^{23}$ cm^{-3} and $n_H = 4 \times 10^{23}$ cm^{-3}.

screening charge to $Z_{scr} = 0.45$ (dots than can be barely seen next to the full solution) to obtain agreement. This has quite an effect, especially, for larger k values used for back-scattering.

Similar results follow for beryllium ions with three bound electrons. Here, the third electron screens the core even further yielding $Z_{scr} = 0.55$ as the best fit for the 1s electrons. The 2s electrons are further out and are best described by an effective charge of $Z_{eff} = 4 - Z_{scr} = 2.55$. However, one can already observe in Fig. 2 that this approach does not yield perfect results and the use of hydrogenic wave functions should be limited to ions with very few bound electrons.

3. Ionic Structure: Multi-Component Hypernetted Chain Equations
We now turn to the calculation of the ionic structure factor in multi-component plasmas. The approach is based on integral equations known from fluid theory that describe the strong coupling between and within the components. The first equation is the Ornstein-Zernicke relation [7]

$$h_{ij}(r) = c_{ij}(r) + \sum_k n_k \int d\bar{r}\, c_{ik}(\bar{r})\, h_{kj}(|r - \bar{r}|) \,. \tag{3}$$

This equation connects the direct correlation functions $c(r)$ with the total correlation function $h(r) = g(r) - 1$, where $g(r)$ is the pair distribution or, in a fluid, the radial distribution function. As a second equation serves the hypernetted chain closure relation

$$g_{ij}(r) = \exp(-\beta V_{ij}(r) + h_{ij}(r) - c_{ij}(r)) \tag{4}$$

which is known to yield reliable results for moderately coupled Coulomb systems [7].

The above system of equations can be solved iteratively. For such a procedure, it is useful to transform the Ornstein-Zernicke relation into Fourier space, where it becomes an algebraic Matrix equation

$$\tilde{H}(k) = \tilde{C}(k) + \tilde{C}(k)\tilde{D}\tilde{H}(k) \,. \tag{5}$$

For the arbitrary number of components considered here, this equation must be solved by numerical matrix inversion for each k value. After rearranging the data into new total correlation functions and a fast Fourier transformation, the closure relation (4) can be used to obtain better direct correlation functions $c(r)$. These functions are in turn transformed back to wave number space and used again in the Ornstein-Zernicke relation (3) until convergence is achieved.

Fig. 3 shows results for a strongly coupled CH_4 plasma, where the electrons are treated within linear response yielding a Debye potential between the ions. As expected, the higher charged
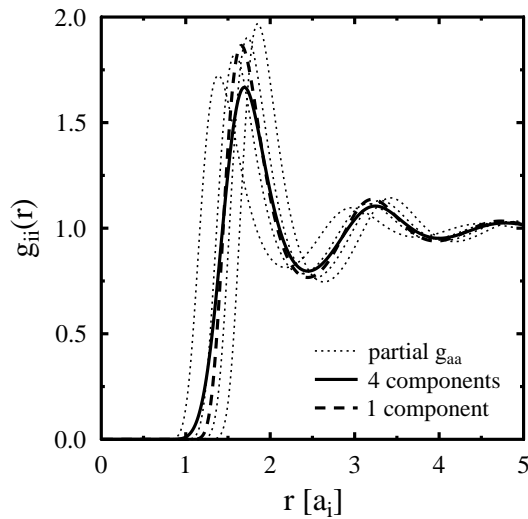
Figure 4. Pair distribution functions for the ions in a partially ionized aluminum plasma with $T = 4 \times 10^3\,\mathrm{K}$ at solid density. The ions have been artificially distributed to four charge states from $Z=1$ to $Z=4$ giving the extremes four times less weight.
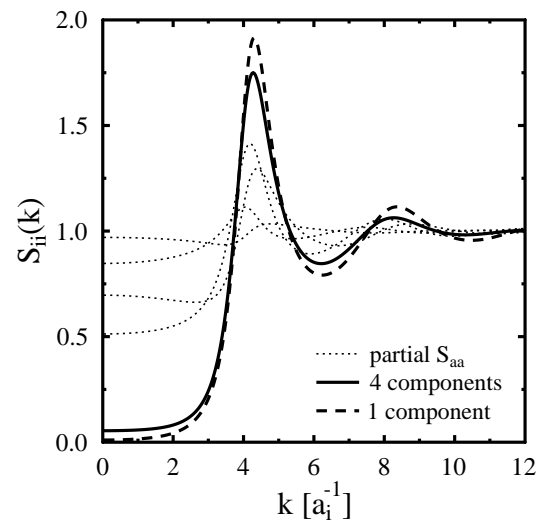

Figure 5. Static structure factor for the ions in an aluminum plasma with the same plasma parameters as in Fig. 4. Note the huge relative difference between the full and the one component calculation at small wave numbers.

carbon ions show a more distinctive structure than the protons or the cross term. However, the proton subsystem by itself would show almost no structure although it has only 20% less ions than the full CH_4 system. This demonstrates the highly correlated behaviour allowing the carbon ions to impose their structure on the protons.

An aluminum plasma with four different charge states is considered in Figs. 4 and 5 which display partial pair distributions and structure factors $S_{ab}(k) = \delta_{ab} + \int [g_{ab}(r) - 1] \exp(-i\mathbf{k}\mathbf{r})\,d\mathbf{r}$, respectively. Again, we consider ions that interact via statically screened forces. The thick full lines show the average over all partial functions. It should be mentioned that all partial g_{ab} lie in between the lines shown. However, S_{ab} for $a \neq b$ displays quite a different behaviour since the Kronecker δ_{ab} is missing in this case. These contributions are also responsable for the fact that the average static structure factor $S(k) = (1/16) \sum_{ab} S_{ab}(k)$ is for small wave numbers k much lower than the partial functions plotted. For comparison, results from an one component calculation for ions with an average charge state of $\bar{Z} = 2.5$ is given. Although both calculations consider the same average charge state, the average pair distributions and static structure factors are quite different; particularly, the experimentally important structure factors at small wave numbers. Accordingly, the ion peak predicted in the total structure factor (2) shows large relative discrepancies.

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