

Static and Dynamic Structure Factors with Account of the Ion Shell Structure for High-temperature Alkaline Earth Plasmas

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The structure and thermodynamic properties of alkali and alkaline earth plasmas are of basic interest and of importance for high-temperature technical applications. For instance, Li is an alkali metal, is planned to be used in inertial confinement fusion, solar power plants etc. In our previous work [1] we studied the two-component plasma (TCP) static (SSF) and dynamic structure factors (DSF) for alkali plasmas. The present study is devoted to the study of the TCP SSF and DSF for alkaline earth (Be^{2+} , Mg^{2+} , Ca^{2+} , Sr^{2+} , Ba^{2+}) plasmas at temperatures $T \geq 200$ kK respectively, where most of outer electrons are ionized, but the rest core electrons are still tightly bound. The structure factor (SF) is the fundamental quantity that describes the X-ray scattering plasma cross-section. Recently, X-ray scattering experiments has proven to be a powerful technique in measuring densities, temperatures, charge states and spectrally resolving the non-collective (particle) scattering characteristics of beryllium [2] in warm dense matter regimes. We follow here the relatively simple analytical route based on Bogolyubov expansions and consider it as an alternative to methods based on *ab initio* quantum DFT molecular dynamic simulations, hypernetted-chain (HNC) etc. Following our method we need for the determination of SSF and DSF a screened pseudopotential as an essential input value. In order to correctly describe alkaline earth plasmas at moderate temperatures one needs to take into account the ion shell structure. In both methods the screened Hellmann-Gurskii-Krasko potential (HGK) $\Phi_{ab}(k)$ ($a, b = i, e$), obtained on the basis of Bogolyubov's method [3], has been used taking into account not only the quantum-mechanical effects (diffraction and symmetry) but also the repulsion due to the Pauli exclusion principle [4] (and references therein). The repulsive part of the HGK potential reflects important features of the ion shell structure. The TCP charge-charge SSF are calculated within the screened HGK approach for one-temperature alkaline earth TCP plasmas at $T = 20\text{eV}$, $\Gamma_{ii} = 0.8$, $n_e = 0.1 \cdot 10^{23} \text{cm}^{-3}$ and $\Gamma_{ii} \approx 2.3$, $n_e = 2.5 \cdot 10^{23} \text{cm}^{-3}$ using the TCP HNC approximation developed for the case of absence of the local thermodynamic equilibrium (non-LTE) by P. Seuferling et al., Phys. Rev. A. 40 (1989), and further discussed and extended for SSF by Gregori et al. [2]. The TCP DSFs for alkaline earth plasmas are calculated within the screened HGK approach at $T = 20\text{eV}$, $\Gamma_{ii} = 0.5$, $n_e = 0.8 \cdot 10^{23} \text{cm}^{-3}$ using the method of moments developed by V. M. Adamyan et al. [5]. Strictly speaking, the model mentioned here based on Bogolyubov expansions is valid only for weakly and moderately coupled plasmas $\Gamma_{ii} \lesssim 1$, $\Gamma_{ii}[ee] = z^2 e^2 [e^2] / (4\pi\epsilon_0 k_B T r_{ii}[ee])$ with $r_{ii}[ee] = (3/4\pi n_i [n_e])^{1/3}$ being the average ion-ion [electron-electron] distance, e is the electric elementary charge and z - the ionic charge, $n_e[i]$ - electron, ion concentrations. We present also the results of several calculations of $\Gamma_{ii} > 1$ but these results have merely the character of extrapolations. The $a - b$ HGK potential has the following view:

$$\varphi_{ab}^{HGK}(r) = \frac{Z_a Z_b}{4\pi\epsilon_0 r} \left[1 - \exp\left(-\frac{r}{R_{Cab}}\right) \right] + \frac{\text{abs}(Z_a Z_b)}{4\pi\epsilon_0} \frac{a}{R_{Cab}} \exp\left(-\frac{r}{R_{Cab}}\right), \quad (1)$$

where $Z_i = ze$, $Z_e = -e$, $R_{Cei} = r_{Cei} r_B$ and a are the pseudopotential parameters. Unfortunately there are no available HGK parameters for the alkaline earth ions. That is why we looked for alternative $e - i$ potentials with the determined for alkaline earth plasmas parameters. It is the C. Fiolhais et al. pseudopotential, Phys. Rev. B 51 (1995). We made a fit of the “universal” parameters of HGK to the Fiolhais et al. pseudopotential, which are Be^{2+} : $a = 3.72$, $r = 0.22$, Mg^{2+} : $a = 2.5$, $r_{Cei} = 0.41$, Ca^{2+} : $a = 1.95$, $r_{Cei} = 0.595$, Sr^{2+} : $a = 1.77$, $r_{Cei} = 0.688$, Ba^{2+} : $a = 1.62$, $r_{Cei} = 0.743$. The $e - e$ interaction is described with the help of the Deutsch potential [4] (and references therein). The values of r_{Cii} , a are not given in literature, therefore $r_{Cii} = 2r_{Cei}$ is taken hypothetically taking in this way both ions cores (closed shells) into account.

Static Structure Factors

The partial SSF of the system are defined as the static (equal-time) correlation functions of the Fourier components of the microscopic partial charge densities, J. P. Hansen, Phys. Rev. A. (1981). A linear combination of the

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partial structure factors which is of high importance, is the charge-charge SSF defined as

$$S_{zz}(k) = \frac{1}{N_e + zN_i} \langle \rho^z(\vec{k})\rho^z(-\vec{k}) \rangle = \frac{S_{ee}(k) - 2\sqrt{z}S_{ei}(k) + zS_{ii}(k)}{z + 1}, \quad (2)$$

where $\rho^z = \rho^i(\vec{k}) - \rho^e(\vec{k})$ with $\rho^r(\vec{k}) = \sum_{i=1}^N \exp(i\vec{k} \cdot \vec{r}_i)$, N_r , $r = e, i$ - number of ions (i) and electrons (e). In the thermodynamic equilibrium (TE) the partial SSF $S_{rs}(k)$ are defined as the Fourier transform of the pair distribution functions $h_{rs}(r) = g_{rs}(r) - 1$: $S_{rs}^{TE}(k) \simeq \delta_{rs} - \frac{\sqrt{n_r n_s}}{k_B T} \Phi_{rs}(k)$, where Φ_{rs} are the expression (11)-(14) in [4].

Introduction of the effective temperature allows to extend the fluctuation-dissipation theorem (FDT) to nonequilibrium (two-temperature) systems as well as to interpolate between classical and quantum regimes and is the input value for the partial SSF $S_{rs}(k)$. The effective temperature T'_{rs} is given by, $T'_{rs} = \frac{m_r T'_s + m_s T'_r}{m_r + m_s}$, where $T'_e = (T_e^2 + T_q^2)^{1/2}$ with $T_q = T_F / (1.3251 - 0.1779\sqrt{r_s})$, where $r_s = r_a/r_B$, $T_F = \hbar^2(3\pi^2 n_e)^{2/3} / (2k_B m_e)$ and $T'_i = (T_i^2 + \gamma_0 T_D^2)^{1/2}$, $T_D = \Omega_{pi} \hbar / k_B$, $\gamma_0 = 0.152$ is the Bohm-Staver relation for the Debye temperature with $\Omega_{pi}^2 = \omega_{pi}^2 / (1 + k_{De}/k^2)$, $\omega_{pi} = \sqrt{ze^2 n_e / (\epsilon_0 m_i)}$ with m_i being the ion mass, $k_{De} = \sqrt{e^2 n_e / (\epsilon_0 k_B T'_e)}$ is the Debye wave number for the electron fluid ($T_D \approx 0.16\text{eV}$, $T_F \approx 14.5\text{eV}$ for Be^{2+}). Due to $m_i \gg m_e$, $T'_{ei} = T'_{ee}$. As described in [2] by Gregori et al., the FDT may still be a valid approximation even under nonequilibrium conditions if the temperature relaxation is slow compared to the electron density fluctuation time scale. A common condition in experimental plasmas for this to occur is when $m_i \gg m_e$ so that the coupling between the two-components takes place at sufficiently low frequencies. Using a two-component HNC approximation scheme, P. Seuferling et al., Phys. Rev. A. 40 (1989), have shown that the static response under the conditions of the non-LTE (two-temperature) takes the form:

$$S_{rs}^{non-LTE}(k) = \delta_{rs} - \frac{\sqrt{n_r n_s}}{k_B T'_{rs}} \Phi_{rs}(k) - \delta_{er} \delta_{es} \left(\frac{T'_e}{T'_i} - 1 \right) \frac{|q(k)|^2}{z} S_{ii}(k) \quad (3)$$

where $q(k) = \sqrt{z}S_{ei}(k)/S_{ii}(k)$. Note that when $T'_e = T'_i = T_e = T_i$ the equation (3) turns into the eq. $S_{rs}^{TE}(k)$ for one-temperature plasma. $q(k)$ represents the screening cloud of free (and valence) electrons that surround the ion. Since the equation (3) represents the HNC-approximation, we will use this approximation for the treatment of non-isothermal (two-temperature), stronger (moderately) coupled plasmas and for comparison with the corresponding results of Gregori et al. All the parameters considered here are beyond the degeneration border ($n_e \lambda_{ee}^3 < 1$).

In Figures 1 (a) - (b) we compare our results on the charge-charge SSF (2) using (3) at $T'_e \simeq T_e = T_i = T'_i$ for alkaline earth plasmas within the screened HGK model with the results obtained in the present work for alkaline earth plasmas considered within the screened Deutsch model for various values of density and fixed temperature. All curves obtained within the screened Deutsch model converge to each other due to the negligible influence of an alkaline earth ion mass on the wavelength λ_{ab} scale entering the equations [2]. As one can easily see with the growth of plasma coupling the peaks become more pronounced and the difference among the curves becomes significant. We see that moderate coupling and the onset of short-range order manifest themselves in S_{zz} as a first localized peak, shown in an amplified scale, also reported in [2], [1] at different values of k' for every alkaline earth species, and with increase of number of shell electrons (from Be^{2+} to Ba^{2+}) the position of the peaks shifts in the direction of small values of k' . We note that our approach is strictly speaking valid only for weakly and moderately coupled plasmas $\Gamma_{ii} \lesssim 1$. The results which we presented here for $\Gamma_{ii} > 1$ have to be considered as extrapolations to a region where the Bogolyubov expansions should include more terms. In Fig. 1 (c) the radial distribution functions (RDF) $g_{ab} \simeq \exp(-\Phi_{ab}(k)/k_B T)$ compared to the hypernetted-chain approximation results obtained by E. Apfelbaum for a Be^{2+} plasma at $n_e \approx 2.5 \cdot 10^{23} \text{cm}^{-3}$, $z \approx 2$, $T_e = 20\text{eV}$, $T'_e \simeq T_e = T_i = T'_i$ is shown. In the HNC calculations the $e - e$, $e - i$ HGK and $e - e$ Deutsch pseudopotentials have been used. One can observe quite satisfactory agreement between the theoretical and HNC results.

The dynamic structure factor: the moment approach

A new “moment approach” based on exact relations and sum rules was suggested in [5]a in order to calculate dynamic characteristics of OCP and of the charge-charge DSF of model semiquantal TCP. This approach proved to produce good agreement with the MD data of J. P. Hansen et al., Phys. Rev. A. (1981). The corresponding DSF are the Fourier transforms of the density-density time correlation functions. Alternatively, the charge-charge DSF

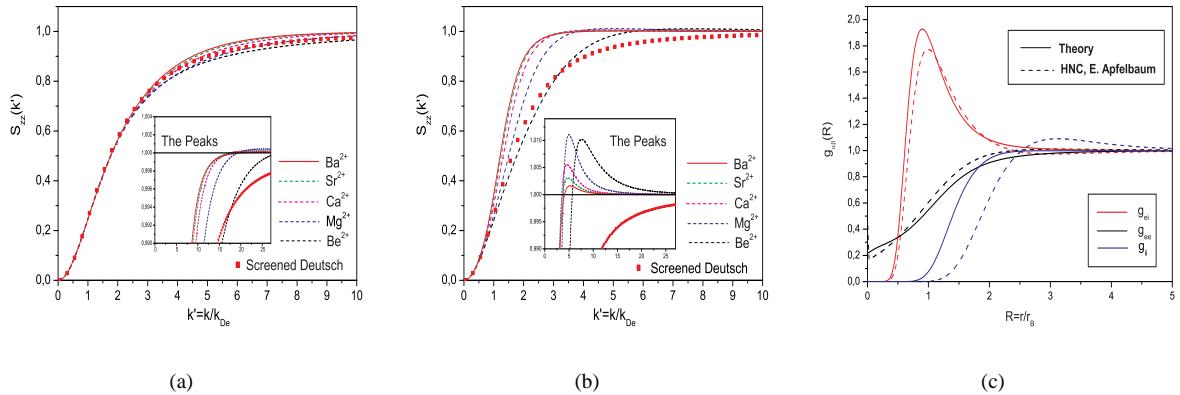


Figure 1: The charge-charge SSF S_{zz} (2), (3) for alkaline earth plasmas at $T'_e \simeq T_e = T_i = T'_i = 20\text{eV}$ (a) $\Gamma_{ii} = 0.8$, (b) $\Gamma_{ii} = 2.3$ and (c) RDF obtained within the screened HGK model for Be^{2+} plasma in comparison with HNC calulations at $n_e \approx 2.5 \cdot 10^{23} \text{cm}^{-3}$, $z \approx 2$ and $T'_e \simeq T_e = T_i = T'_i = 20\text{eV}$. In the (a), (b) the present results are compared with those obtained in the present work for alkaline earth plasmas in a frame of the screened Deutsch model on a base of Gregori et al.[2]. In the (c) the set of solid lines represents the present theoretical results within the screened HGK model, while the set of dashed lines - HNC results obtained by E. Apfelbaum within the HGK $e - i$ and $i - i$ and Deutsch $e - e$ pseudopotential models. As the length scale we use the inverse electron Debye radius.

$S_{zz}(k, \omega)$ can be defined via the FDT [5]b as

$$S_{zz}(k, \omega) = -\frac{\hbar \text{Im} \varepsilon^{-1}(k, \omega)}{\pi \Phi(k) [1 - \exp(-\beta \hbar \omega)]}, \quad (4)$$

where $\Phi(k) = z^2 e^2 / \varepsilon_0 k^2$ and $\varepsilon^{-1}(k, \omega)$ is the inverse longitudinal dielectric function of the plasma.

On a base of the Nevanlinna formula of the classical theory of moments [5]b (and references therein), we calculate the relative charge-charge DSF takes the following form:

$$\frac{S_{zz}(k, \omega)}{S_{zz}(k, 0)} = \frac{\beta \hbar}{[1 - \exp(-\beta \hbar \omega)]} \times \frac{\omega h^2(k) \omega_1^4}{\omega^2(\omega^2 - \omega_2^2) + h^2(k)(\omega^2 - \omega_1^2)} \quad , \quad h(k) = \frac{(\omega_2^2 - \omega_1^2) \omega_p^2}{\pi \beta \phi(k) \omega_1^4 S_{zz}(k, 0)} > 0 \quad (5)$$

with $S_{zz}(k, 0) \simeq S_{zz}^0(k, 0) = \frac{n_e}{k} \sqrt{\frac{m}{2\pi k_B T}}$, $\omega_1^2 = C_2/C_0 = \omega_p^2 [1 - \varepsilon^{-1}(k, 0)]^{-1}$, $\omega_2^2 = C_4/C_2 = \omega_p^2 [1 + Q(k)]$, where $\varepsilon^{-1}(k, 0)$ can be determined from eq. (4) at $\hbar = 0$ and Kramers-Kronig relation as $\text{Re} \varepsilon^{-1}(k, 0) = 1 - 2S_{zz}(k)k_{De}^2/k^2$, where $\text{Re} \varepsilon^{-1}(k, 0) = \varepsilon^{-1}(k, 0) = \varepsilon^{-1}(k)$ and $S_{zz}(k)$ is defined at $T'_e = T'_i = T_e = T_i$ by (2), (3) or $S_{rs}^{TE}(k)$. The function defining the second moment is given by $Q(k) = K(k) + L(k) + H$ [5]b. It contains the kinetic contribution for a classical system $K(k) = 3k^2/k_D^2$, where $k_D^2 = k_{De}^2 = n_e e^2 / \varepsilon_0 k_B T$. The Nevanlinna method does not fix the function $h(k)$ up to some requirements as e.g. $h(k) > 0$. We are using this freedom and chose expression for $H(k)$, $L(k)$. That is why we use for comparison two definitions: using the Coulomb and HGK interactions. The contribution due to electron-ion Coulomb [6] and HGK correlations are in our approach represented respectively by :

$$H^C = \frac{4}{3} z r_s \sqrt{\Gamma_{ee}} [3z \Gamma_{ee}^2 + 4r_s + 4\Gamma_{ee} \sqrt{3(1+z)r_s}]^{-1/2} \quad , \quad H^{HGK} = \frac{h_{ei}(r=0)}{3} = \frac{g_{ei}(r=0) - 1}{3} = -\frac{1}{3} \quad (6)$$

The term $L(k)$ takes into account the $e - e$ Coulomb and HGK correlations respectively:

$$L^{C, HGK}(k) = \frac{1}{2\pi^2 n_e} \int_0^\infty p^2 [S_{ee}(p) - 1] f(p, k) dp, \quad (7)$$

$$f^C(p, k) = \frac{5}{12} - \frac{p^2}{4k^2} + \frac{(k^2 - p^2)^2}{8pk^3} \ln \left| \frac{p+k}{p-k} \right|, \quad f^{HGK}(p, k) = \int_{-1}^1 \frac{(ps-k)^2}{p^2 - 2psk + k^2} \zeta_{ee}(\sqrt{p^2 - 2pks + k^2}) \frac{ds}{2} - \frac{\zeta_{ee}(p)}{3} \quad (8)$$

where $\zeta_{ee}(p)$ is to be determined from the Deutsch potential $\varphi_{ee}(p) = \Phi(p)\zeta'_{ee}(p)$, where $\Phi(p) = 4\pi e^2/4\pi\epsilon_0 p^2$ - Fourier transform of the Coulomb potential.

In Figure 2 the DSF with the different definitions of H^H , L^C in the (a) and H^{HGK} , L^{HGK} in the (b), (6) and

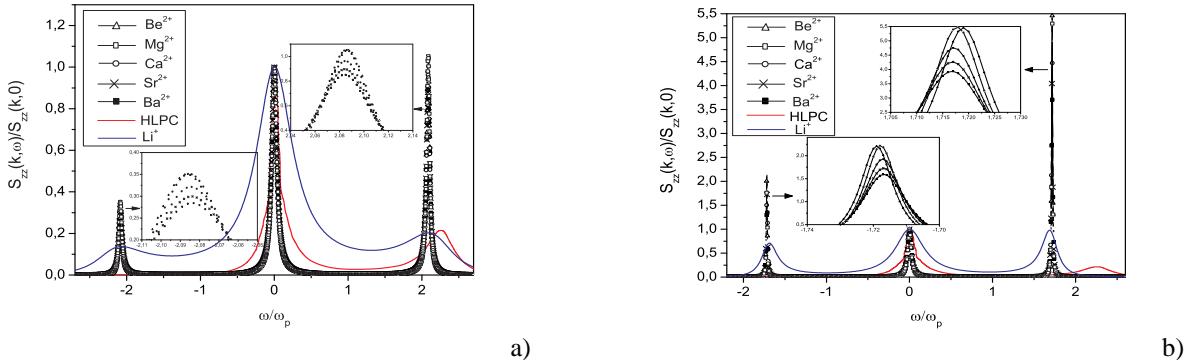


Figure 2: Comparisons of the relative charge-charge DSFs (5) of alkaline earth plasmas at $\Gamma_{ee} = 0.5$ and $T = 232090K$, $n_e = 0.8 \cdot 10^{23} cm^{-3}$ with the results obtained in [1] for Li^+ plasma at $T = 30000K$, $n_e = 1.741 \cdot 10^{20} cm^{-3}$ and obtained by S. Adamjan et al. in [5]b at $T = 1574573K$, $n_e = 2.5 \cdot 10^{25} cm^{-3}$ for the HLPC model at $k = 1.074 \cdot r_{ee}$, (a) H^H , L^C and (b) H^{HGK} , L^{HGK} are defined as (6) and (7), (8). As the length scale we use the electron plasma frequency $\omega_p = n_e e^2 / \epsilon_0 m_e$.

(7), (8) respectively, are shown for comparison with the HLPC model in [5]b and alkali Li^+ plasma. As one can see in the Figures the curves for alkaline earth plasmas are different from those given for the HLPC model [5]b, Li^+ plasma as well as they are in comparison with each other. The differences are due to the repulsive parts of the HGK potential, compared to the HLPC model, which reflects roughly the internal ion shell structure. In our previous work [1] we showed that at higher Γ_{ii} alkali ion shell structure influences the dynamic structure factor significantly leading to the splitting of the DSF curves with respect to every species. Here we could not consider the results at the same $\Gamma_{ii} = 2$ as used by Adamyan et al.[5]b because plasma becomes degenerate. In the Figures the position of the central peaks coincides but positions of the plasmon peaks compared to the HLPC model are slightly shifted. In alkaline earth plasmas the plasmon peaks are more pronounced compared to the Li^+ and HLPC plasma especially in the Fig. 2 (b) where the ion shell structure is better taken into account through H^{HGK} , L^{HGK} . This can be explained by stronger $i - i$ interaction ($\Gamma_{ii} = 1.56$) in comparison with the alkali and HLPC ions, where $\Gamma_{ii} = 0.5$. We observe that the plasmon peaks in the Fig. 2 (b) are shifted in the direction of smaller absolute value of ω/ω_p and the heights of the plasmon peaks are higher then in the Fig. 2 (a). All this could be explained by some coupling between bound electrons and the plasmon mode. Observe that in both cases 2 (a), (b) with an increase of number of shell electrons from Be^{2+} to Ba^{2+} the curves shift in the direction of low absolute value of ω/ω_p and their heights diminish. The difference is due to the short range forces which we took into account by the HGK model in comparison with the HLPC model. One should also take into account that we employed different plasma parameters because at the high densities and temperatures studied in [5]b inner electron shells of the alkaline earth plasmas are destroyed.

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