Static and Dynamic Structure Factors with Account of the Ion Structure for High-temperature Alkali and 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. The present study is devoted to the study of the two-component plasma (TCP) static (SSF) and dynamic (DSF) structure factors for alkali (Li^+, Na^+, K^+, Rb^+, Cs^+) and alkaline earth (Be^{2+}) plasmas at temperatures $T \geq 30$ kK and $T \geq 100$ 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 [1] 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 alkali plasmas at moderate temperatures one needs to take into account the ion 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 [2], 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 [3] and references therein. The repulsive part of the HGK potential reflects important features of the ion structure. The TCP electron-electron , electron-ion, ion-ion and charge-charge static structure factors are calculated within the HGK approach for alkali one-temperature plasma at $T = 30000K$, $n_e = 0.3 \cdot 10^{21} \div 1.9 \cdot 10^{22} cm^{-3}$ and charge-charge SSF for Be^{2+} TCP at $T = 20eV$, $n_e = 2.5 \cdot 10^{23} cm^{-3}$ 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. [1] . The TCP DSFs for alkali plasmas are calculated within the HGK approach at $T = 30000K$, $n_e = 1.74 \cdot 10^{20}, 1.11 \cdot 10^{22} cm^{-3}$ using the method of moments developed by V. M. Adamyan et al. [4]. Strictly speaking, the model mentioned here based on Bogolyubov expansions is valid only for weakly and moderately coupled plasmas $\Gamma_{ii} \lesssim 1$, $\Gamma_{ii}[_{ee}] = z^2 e^2 [e^2]/(4\varepsilon_0 k_B T r_{ii}[_{ee}])$ 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:

$$\varphi^{HGK}{}_{ab}(r) = \frac{Z_a Z_b}{4\pi\varepsilon_0 r}\left[1 - \exp\left(-\frac{r}{R_{Cab}}\right)\right] + \frac{abs(Z_a Z_b)}{4\pi\varepsilon_0}\frac{a}{R_{Cab}}\exp\left(-\frac{r}{R_{Cab}}\right), \tag{1}$$

where $Z_i = ze$, $Z_e = -e$, $R_{Cei} = r_{Cei} r_B$ and a for alkali elements are taken from [3] 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. Unfortunately there are no available HGK parameters for the Be^{2+} ion. That is why we looked for alternative $e-i$ potentials with the determined for Be^{2+} 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 $a = 3.72$, $r = 0.22$. The $e-e$ interaction is described with the help of the Deutsch potential [3] and references therein.

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

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

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where $\rho^z = \rho^i(\vec{k}) - \rho^e(\vec{k})$ with $\rho^r(\vec{k}) = \sum_{i=1}^{N} \exp(\imath\vec{k}\cdot\vec{r}_i^r)$, N_r, $r = e,i$- number of ions (i) and electrons (e). In the thermodynamic equillibrium (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 [3].

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 $\Omega_{pi}^2 = \omega_{pi}^2/(1 + k_{De}/k^2)$, $\omega_{pi} = \sqrt{ze^2 n_e/(\varepsilon_0 m_i)}$ with m_i being the ion mass, $k_{De} = \sqrt{e^2 n_e/(\varepsilon_0 k_B T'_e)}$ is the Debye wave number for the electron fluid ($T_D \approx 0.16eV$, $T_F \approx 14.5eV$ for Be^{2+}). Due to $m_i >> m_e$, $T'_{ei} = T'_{ee}$. As described in [1] 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 $m_i >> m_e$ 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:

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

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 $T'_e = T'_i = T_e = T_i$ for alkali plasmas within the screened HGK model with the results obtained in the present work for alkali (hydrogen-like point charges (HLPC)) 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 alkali ion mass on the wavelength λ_{ab} scale entering the equations [1]. As one can easily see with the growth of 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 [1], at different values of k' for every alkali species, and with increase of number of shell electrons (from Li^+ to Cs^+) 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 SSFs (2) for a Be^{2+} plasma with $n_e \approx 2.5 \cdot 10^{23} cm^{-3}$, $z \approx 2$, $T_e = 20eV$ and $T_i = T_e$, $T_i = 0.5 \cdot T_e$, $T_i = 0.2 \cdot T_e$ are shown.

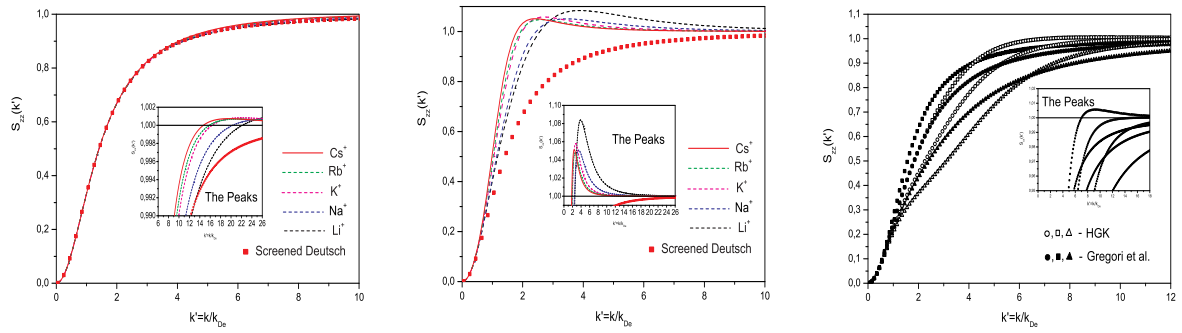
The dynamic structure factor: the moment approach

A new "moment approach" based on exact relations and sum rules was suggested in [4]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 $S_{zz}(k,\omega)$ can be defined via the FDT [4]b as

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

where $\Phi(k) = e^2/\varepsilon_0 k^2$ 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 [4]b and references therein, we calculate



(a) (b) (c)

Figure 1: The charge-charge SSF S_{zz} (2), (3) for alkali plasmas at $T_e = T_i = T_e' = T_i' = 30000K$ (a) $\Gamma_{ii} = 0.6$, (b) $\Gamma_{ii} = 2.4$ and (c) for Be^{2+} plasma with $n_e \approx 2.5 \cdot 10^{23} cm^{-3}$, $z \approx 2$, and $T_e = 20eV$, $T_e' = 24.06eV$ in a frame of the screened HGK model. In the (a), (b) the present results are compared with those obtained in the present work for HLPC plasmas in a frame of the screened Deutsch model on a base of Gregori et al.[1]. In the (c) the set of filled symbols represents the HLPC model obtained by Gregori et al.[1], while the set of hollow symbols - the screened HGK model. Squares: $T_i/T_e = 1$ ($\Gamma_{ii} = 2.31$, $\Gamma_{ee} = 0.61$). Circles: $T_i/T_e = 0.5$ ($\Gamma_{ii} = 4.63$, $\Gamma_{ee} = 0.61$). Triangles: $T_i/T_e = 0.2$ ($\Gamma_{ii} = 11.57$, $\Gamma_{ee} = 0.61$).the solid line: $T_i/T_e = 1$ ($\Gamma_{ii} = 2.31$, $\Gamma_{ee} = 0.61$). Dashed line: $T_i/T_e = 0.5$ ($\Gamma_{ii} = 4.63$, $\Gamma_{ee} = 0.61$). Dotted line: $T_i/T_e = 0.2$ ($\Gamma_{ii} = 11.57$, $\Gamma_{ee} = 0.61$). As the length scale we use the inverse electron Debye radius.

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 $S_{zz}(k,0) \simeq S^0_{zz}(k,0) = \frac{n_e}{k}\sqrt{\frac{m}{2\pi k_B T}}$, ${\omega_1}^2 = C_2/C_0 = {\omega_p}^2[1-\varepsilon^{-1}(k,0)]^{-1}$, ${\omega_2}^2 = C_4/C_2 = {\omega_p}^2[1+Q(k)]$, where $\varepsilon^{-1}(k,0)$ can be determined from eq. (4) at $\hbar = 0$ and Kramers-Kronig relation as $Re\varepsilon^{-1}(k,0) = 1 - 2S_{zz}(k){k_{De}}^2/k^2$, where $Re\varepsilon^{-1}(k,0) = \varepsilon^{-1}(k,0) = \varepsilon^{-1}(k)$ and $S_{zz}(k)$ is defined at $T_e' = T_i' = T_e = T_i$ by (2), (3) or $S^{TE}_{rs}(k)$. The function defining the second moment is given by $Q(k) = K(k) + L(k) + H$ [4]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 (for Hydrogen [5]) and HGK correlations are in our approach represented respectively by :

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

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

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

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

where $\zeta_{ee}(p)$ is to be determined from the Deutsch potential $\varphi_{ee}(p) = \Phi(p)\zeta_{ee}'(p)$, where $\Phi(p) = 4\pi e^2/4\pi\varepsilon_0 p^2$ - Fourier transform of the Coulomb potential.

In Figure 2 the DSF with the different definitions of H^H, L^C in the (a), (b) and H^{HGK}, L^{HGK} in the (c), (d), (6) and (7), (8) respectively, are shown for comparison with the HLPC model in [4]b. As one can see in the Figures the curves for alkali plasmas are different from those given for the HLPC model [4]b 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,

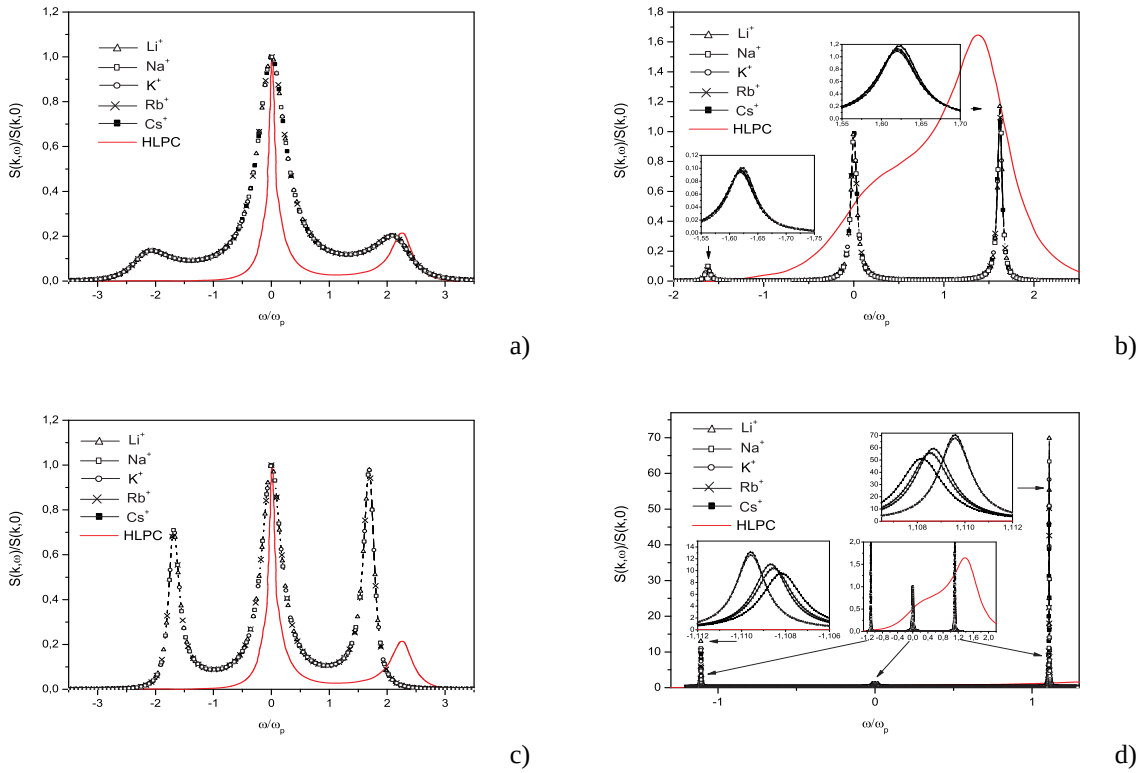


Figure 2: Comparisons of the relative charge-charge DSFs (5) of alkali plasmas with the results obtained by S. Adamjan et al. [4]b for the HLPC model at $T = 30000K$, $k = 1.074 \cdot r_{ee}$, (a), (c) $n_e = 2.5 \cdot 10^{25} cm^{-3}$, $\Gamma_{ee} = 0.5$ and (b), (d) $n_e = 1.61 \cdot 10^{24} cm^{-3}$, $\Gamma_{ee} = 2$, where in the (a), (b) H^H, L^C and (c), (d) H^{HGK}, L^{HGK} are defined as (6) and (7), (8). As the length scale we use the electron plasma frequency $\omega_p = n_e e^2/\varepsilon_0 m_e$.

which reflects roughly the internal ion structure. In the case of alkali plasmas at higher Γ_{ii} the curves split. This can be explained by that fact that at higher Γ_{ii} alkali ion structure influences the dynamic structure factor significantly. In the Figures the position of the central peaks coincides but positions of the plasmon peaks are slightly shifted . In alkali plasmas the plasmon peaks are more pronounced especially in the Fig. 2 (c), (d) where the ion structure is better taken into account through H^{HGK}, L^{HGK}. We observe that the plasmon peaks in the Fig. 2 (c), (d) are more pronounced and shifted in the direction of smaller absolute value of ω/ω_p, the heights of the plasmon peaks are higher especially at higher Γ_{ii} then in the Fig. 2 (a), (b). All this could be explained by some coupling between bound electrons and the plasmon mode. Observe that at higher Γ_{ii} with an increase of number of shell electrons from Li^+ to Cs^+ 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 [4]b inner electron shells of the alkali plasmas are destroyed.

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