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

S. P. Sadykova [1], W. Ebeling [1], I.M. Tkachenko [2]

Humboldt-Universität zu Berlin, Germany [1], Universidad Politécnica de Valencia, Camino de Vera, 46022 Spain [2]

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Static structure factors in thermal equilibrium plasmas I

- The partial static structure factors (SSF) $S_{rs}(k)$ of the system are defined as [1]:

$$S_{rs}(k) = \frac{1}{N_i} < \rho^r(\vec{k})\rho^s(-\vec{k}) >, \tag{1}$$

with the microscopic partial charge densities

$$\rho^r(\vec{k}) = \sum_{i=1}^{N_r} \exp\left(\imath \vec{k} \cdot \vec{r}_i^{\,r}\right). \tag{2}$$

$(r, s = e$ (electrons) or i (ions))

The partial SSF are related to screened effective potentials as

$$S_{rs}(k) = \delta_{rs} - \frac{\sqrt{n_r n_s}}{k_B T} \Phi_{rs}(k), \tag{3}$$

Static structure factors in thermal equilibrium plasmas II

where for Φ_{rs} the screened Hellmann-Gurskii-Krasko pseudopotential taking into account the ion shell structure has been used [3]. The Hellmann-Gurskii-Krasko pseudopotentials has the following view:

$$\varphi_{ab}(r) = \frac{e_a e_b}{4\pi\varepsilon_0}\left(\frac{1 - e^{-r/R_{c\,ab}}}{r}\right) + \frac{|e_a e_b|}{4\pi\varepsilon_0}\frac{a}{R_{c\,ab}} e^{-r/R_{c\,ab}}, \qquad (4)$$

where $R_{C\,ab} = r_{c\,ab} r_B$, R_C is the shell size.
The screening effects were incorporated on a base of the classical Bogoljubov's approach [2].

Static structure factors in thermal equilibrium plasmas III

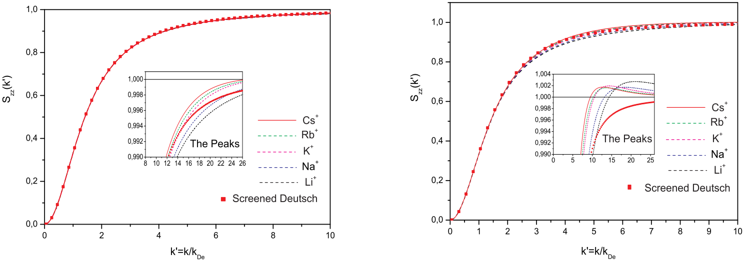
- The effective response of the medium is described by

The charge-charge structure factor

$$S_{zz}(k) = \frac{1}{N_e + N_i} < \rho^z(\vec{k})\rho^z(-\vec{k}) >$$
$$= \frac{S_{ee}(k) - 2\sqrt{z}S_{ei}(k) + zS_{ii}(k)}{1+z}, \quad (5)$$

where z is an ion charge and $\rho^z = \rho^i(\vec{k}) - \rho^e(\vec{k})$.

Static structure factors in thermal equilibrium plasmas IV



a) b)

Figure: The charge-charge static structure factors S_{zz} (5) for alkali plasmas (Li^+, Na^+, K^+, Rb^+, Cs^+) within the HGK model as compared to our results obtained in the present work for hydrogen-like point charges (HLPC) within the Deutsch model on a basis of (5) at $T_e = T_i$. (a) $T_e = 60000K$, $\Gamma_{ee} = 0.398$, $\Gamma_{ii} = 0.399$; (b) $T_e = 30000K$, $\Gamma_{ee} = 0.789$, $\Gamma_{ii} = 0.8$; As scale of the k-vector we use the inverse electron Debye radius k_{De} [4].

Static structure factors in thermal equilibrium plasmas V

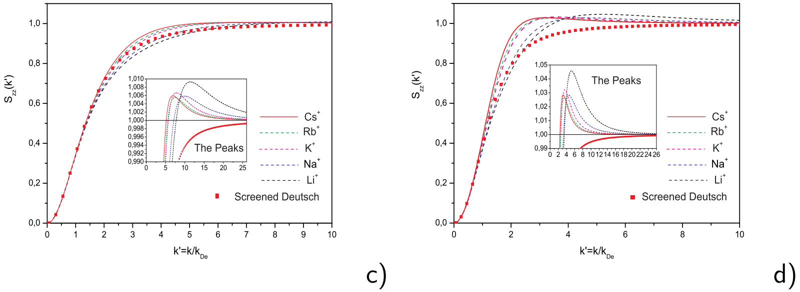


Figure: The charge-charge static structure factors S_{zz} (5) for alkali plasmas (Li^+, Na^+, K^+, Rb^+, Cs^+) within the HGK model as compared to our results obtained in the present work for hydrogen-like point charges (HLPC) plasmas within the Deutsch model on a basis of (5) at $T_e = T_i$. c) $T_e = 30000K$, $\Gamma_{ee} = 1.14$, $\Gamma_{ii} = 1.2$; (d) $T_e = 30000K$, $\Gamma_{ee} = 1.58$, $\Gamma_{ii} = 2$. As scale of the k-vector we use the inverse electron Debye radius k_{De} [4].

Static structure factors for two temperature plasmas I

Using a two-component hypernetted-chain (HNC) approximation scheme, Seuferling et al. [5] have shown that

the partial SSFs under the conditions of the non-LTE (two-temperature) take the form

$$S_{rs}(k) = \delta_{rs} - \frac{\sqrt{n_r n_s}}{k_B T'_{rs}} \Phi_{rs}(k) - \delta_{er}\delta_{es}\left(\frac{T'_e}{T'_i} - 1\right)\frac{|q(k)|^2}{z} S_{ii}(k) \tag{6}$$

where $q(k)$ represents the screening cloud of free (and valence) electrons that surround the ion

$$q(k) = \frac{\sqrt{z} S_{ei}(k)}{S_{ii}(k)}, \tag{7}$$

and for Φ_{rs} the Hellmann-Gurskii-Krasko pseudopotentials (HGK) were used. The effective temperature T'_{rs} is given by,

$$T'_{rs} = \frac{m_r T'_s + m_s T'_r}{m_r + m_s},$$

Static structure factors for two temperature plasmas II

Here $T_e' = (T_e^2 + T_q^2)^{1/2}$ with $T_q = T_F/(1.3251 - 0.1779\sqrt{r_s})$, where $r_s = r_a/r_B$ is the Brueckner parameter, $T_F = \hbar^2(3\pi^2 n_e)^{2/3}/(2k_B m_e)$ 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 definition for the Debye temperature with $\Omega_{pi}^2 = \omega_{pi}^2/(1 + k_{De}/k^2)$, $\omega_{pi} = \sqrt{ze^2 n_e/(\varepsilon_0 m_i)}$, m_i is the ion mass, $k_{De} = \sqrt{e^2 n_e/(\varepsilon_0 k_B T_e')}$ is the electronic Debye wavenumber ($T_D \approx 0.16eV$, $T_F \approx 14.5eV$ for Be^{2+}).

The de Broglie wavelength becomes $\lambda_{rs} = \hbar/\sqrt{2\pi\mu_{rs}' k_B T_{rs}'}$.

Static structure factors for two temperature plasmas III

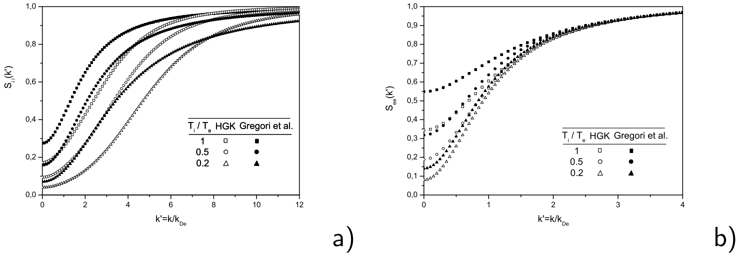


Figure: Static structure factors (6) and the screening charge $q(k')$ for Be^{2+} plasma at $T_e = 20eV$, $T_e' = 24.06eV$, $z = 2$ and $n_e = 2.5 \times 10^{23} cm^{-3}$. The filled symbols represent the screened Deutsch model obtained by Gregori et al. [6], [7], while the empty symbols correspond to 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: $T_i/T_e = 0.2$ $(\Gamma_{ii} = 11.57, \Gamma_{ee} = 0.61)$ [4] $(n_e\lambda_{ee}^3 < 1)$

Static structure factors for two temperature plasmas IV

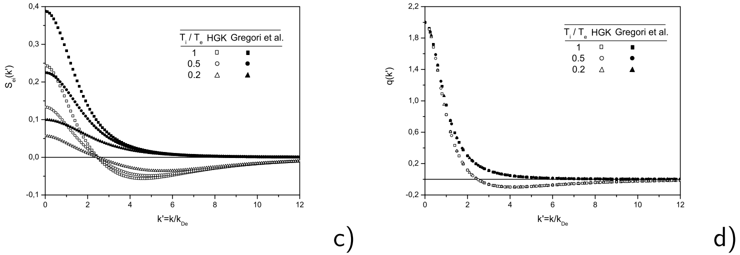


Figure: Static structure factors 6 and the screening charge $q(k')$ for Be^{2+} plasma at $T_e = 20eV$, $T_e' = 24.06eV$, $z = 2$ and $n_e = 2.5 \times 10^{23} cm^{-3}$. The filled symbols represent the screened Deutsch model obtained by Gregori et al. [6], [7], while the empty symbols correspond to 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: $T_i/T_e = 0.2$ ($\Gamma_{ii} = 11.57$, $\Gamma_{ee} = 0.61$) [4] ($n_e \lambda_{ee}^3 < 1$).

Static structure factors for two temperature plasmas V

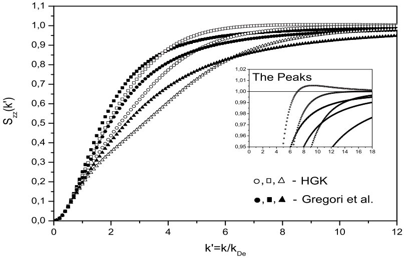


Figure: The charge-charge static structure factors S_{zz} (5) with (6) for a beryllium plasma with $n_e \approx 2.5 \cdot 10^{23} cm^{-3}$, $z \approx 2$, and $T_e = 20eV$, $T_e' = 24.06eV$. The filled symbols represent the screened Deutsch model obtained on the basis of [7] , while the empty symbols correspond to 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: $T_i/T_e = 0.2$ $(\Gamma_{ii} = 11.57, \Gamma_{ee} = 0.61)$ [4].

The dynamic structure factor: the moment approach I

- The partial dynamic structure factors (DSF) $S_{rs}(k)$ of the system are defined as [1]:

$$S_{rs}(k,\omega) = \frac{1}{2\pi N}\int e^{\imath\omega t} < \rho^r(\vec{k},t)\rho^s(-\vec{k},0) > dt. \qquad (8)$$

with the time dependent microscopic partial charge densities

$$\rho^r(\vec{k},t) = \sum_{i=1}^{N} \exp\left(\imath\vec{k}\cdot\vec{r}_i^{\,r}(t)\right). \qquad (9)$$

We employ the method of moments suggested by V.M. Adamjan et. al. [8, 10] which proved to provide a good agreement with the numerical simulation data for of one- and two-component plasmas [1].
The plasma is in a complete thermal equilibrium. The Hydrogen-like Point Charges model, except the static characteristics determined within the HGK model, is applied to determine the moments or the sum rules.

The dynamic structure factor: the moment approach II

- The charge-charge dynamic structure factor $S_{zz}(k,\omega)$ is defined via the fluctuation-dissipation theorem (FDT) as

$$S_{zz}(k,\omega) = -\frac{\hbar Im \varepsilon^{-1}(k,\omega)}{\pi\Phi(k)[1-\exp(-\beta\hbar\omega)]}, \quad (10)$$

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

The charge-charge DSF is directly related to the charge-charge SSF as:

$$\begin{aligned} S_{zz}(k) &= \frac{1}{n_e+n_i}\int_{-\infty}^{\infty} S_{zz}(k,\omega)d\omega \\ &= \frac{S_{ee}(k) - 2\sqrt{z}S_{ei}(k) + zS_{ii}(k)}{z+1}, \end{aligned} \quad (11)$$

where $T'_e = T'_i = T_e = T_i$, $T'_{ei} = T'_{ee} = T'_e$, $n_e = zn_i$ ($z = 1$ for hydrogen-like plasmas).

The dynamic structure factor: the moment approach III

- In order to construct the inverse longitudinal dielectric function within the moment approach one has to consider the frequency moments of the loss function $-Im\varepsilon^{-1}(k,\omega)/\omega$:

$$C_\nu(k) = -\pi^{-1}\int_{-\infty}^{\infty}\omega^{\nu-1} Im\varepsilon^{-1}(k,\omega)d\omega, \qquad (12)$$

  here with $\nu = 0, 2, 4$. The odd-number moments vanish due to the parity of the loss function and that the moment $C_2 = \omega_p^2$ expresses the f-sum rule, ω_p being the plasma frequency.

- Then the Nevanlinna formula of the classical theory of moments [11] expresses the response function

$$\varepsilon^{-1}(k,\omega) = 1 + \frac{{\omega_p}^2(\omega+q)}{\omega(\omega^2-{\omega_2}^2)+q(\omega^2-{\omega_1}^2)}, \qquad (13)$$

  in terms of a Nevanlinna-class $q = q(k,\omega)$ such that

$$\lim_{z\to\infty}\frac{q\,(k,z)}{z} = 0 \quad , \quad Imz \geq 0.$$

The dynamic structure factor: the moment approach IV

- The frequencies ω_1 and ω_2 are defined as respective ratios of the moments C_ν:

$$\omega_1{}^2 = C_2/C_0 = \omega_p{}^2[1-\varepsilon^{-1}(k,0)]^{-1},$$
$$\omega_2{}^2 = C_4/C_2 = \omega_p{}^2[1+Q(k)], \qquad (14)$$

- where $\varepsilon^{-1}(k,0)$ can be determined from the classical form ($\hbar \to 0$) of the FDT (thermal equillibrium) eq. (10) and the Kramers-Kronig relation :

$$Re\varepsilon^{-1}(k,\omega) = 1 + \frac{1}{\pi} P.V. \int_{-\infty}^{\infty} \frac{Im\varepsilon^{-1}(k,\omega)}{\omega' - \omega} d\omega' \qquad (15)$$

In this way, we get the following expression :

$$Re\varepsilon^{-1}(k,0) = 1 - 2S_{zz}(k)\frac{k_{De}{}^2}{k^2}, \qquad (16)$$

where $Re\varepsilon^{-1}(k,0) = \varepsilon^{-1}(k,0) = \varepsilon^{-1}(k)$, $S_{zz}(k)$ is defined by (11).

The dynamic structure factor: the moment approach V

- The function defining the fourth moment is given in the Coulomb HLPC approximation except the static characteristics, given within the HGK model, by [10]:

$$Q(k) = K(k) + L(k) + H. \tag{17}$$

It contains the kinetic contribution, particularly, for a classical system:

$$K(k) = 3\left(\frac{k}{k_D}\right)^2, \tag{18}$$

where ${k_D}^2 = {k_{De}}^2$.
We approximate here the contribution due to the electron-ion correlations by the expression for hydrogen within the modified RPA:

$$H = \frac{4}{3} r_s \sqrt{\Gamma}_{ee} [3\Gamma_{ee}^2 + 4r_s + 4\Gamma_{ee}\sqrt{6r_s}]^{-1/2} \tag{19}$$

The dynamic structure factor: the moment approach VI

Finally, the contribution $L(k)$ takes into account the electronic correlations, we calculated it for the Coulomb potential:

$$L(k) = \frac{1}{2\pi^2 n_e} \int_0^\infty p^2 [S_{ee}(p) - 1] f(p,k) dp, \tag{20}$$

where

$$f(p,k) = \frac{5}{12} - \frac{p^2}{4k^2} + \frac{\left(k^2 - p^2\right)^2}{8pk^3} \ln \left| \frac{p+k}{p-k} \right| . \tag{21}$$

In (20) the static structure factor is the one defined in (6) with the screened e-e HGK potential.

The authors of [10] suggested to approximate $q(k,\omega)$ by its static value $q(k,0) = \imath h(k)$, connected to the static value $S_{zz}(k,0)$ of the dynamic structure factor through eq. (10):

$$h(k) = \frac{({\omega_2}^2 - {\omega_1}^2){\omega_p}^2}{\pi\beta\phi(k){\omega_1}^4 S_{zz}(k,0)} > 0, \tag{22}$$

The dynamic structure factor: the moment approach VII

with $S^0_{zz}(k,0) = \frac{n_e}{k}\sqrt{\frac{m}{2\pi k_B T}}$ so that

the relative dynamic structure factor takes the following form:

$$\frac{S_{zz}(k,\omega)}{S_{zz}(k,0)} = \frac{\beta\hbar}{[1-\exp(-\beta\hbar\omega)]} \times \frac{\omega h^2(k)\omega_1{}^4}{\omega^2(\omega^2-\omega_2{}^2)+h^2(k)(\omega^2-\omega_1{}^2)}, \quad (23)$$

with the more simplified expressions for $h(k)$:

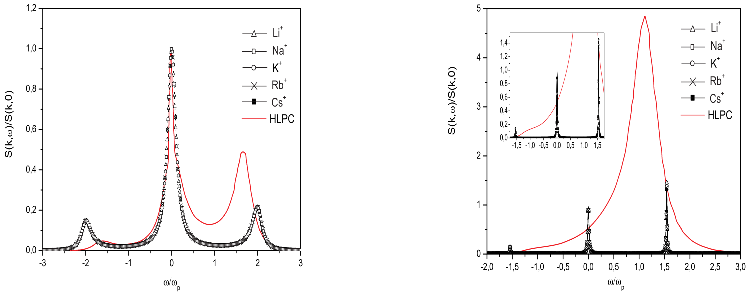
$$h(k) = \frac{\varepsilon_0\sqrt{2\pi k_B T}k^3\omega_p{}^2(\omega_2{}^2-\omega_1{}^2)}{\pi\beta\sqrt{m}n_e e^2\omega_1{}^4}, \quad (24)$$

The dynamic structure factor: the moment approach VIII

and the characterisitic frequencies $\omega_1(k)$, $\omega_2(k)$:

$$\begin{aligned} {\omega_1}^2 &= C_2/C_0 = \frac{{\omega_p}^2 k^2}{2{k_{De}}^2 S_{zz}(k)}, \\ {\omega_2}^2 &= C_4/C_2 = {\omega_p}^2[1 + K(k) + L(k) + H], \end{aligned} \tag{25}$$

The dynamic structure factor: the moment approach IX



a) b)

Figure: The relative charge-charge DSFs of alkali plasmas determined within the HLPC model but with the HGK static characteristics in comparison with the results of [10] obtained within the same HLPC model but with the Coulomb static characteristics at $k = 0.767/r_{ee}$, (a) $\Gamma_{ii} = 0.5$, Present results: $T = 30000K$, $n_e = 1.741 \cdot 10^{20} cm^{-3}$, Adamjan et al.: $T = 1574573K$, $n_e = 2.5 \cdot 10^{25} cm^{-3}$ and (b) $\Gamma_{ii} = 2$, Present results: $T = 30000K$,

The dynamic structure factor: the moment approach X

$n_e = 1.11 \cdot 10^{22} cm^{-3}$, Adamjan et al.: $T = 157457K$, $n_e = 1.61 \cdot 10^{24} cm^{-3}$.
As the frequency scale we use the electron plasma frequency
$\omega_p = \sqrt{n_e e^2/\varepsilon_0 m_e}$ [4].

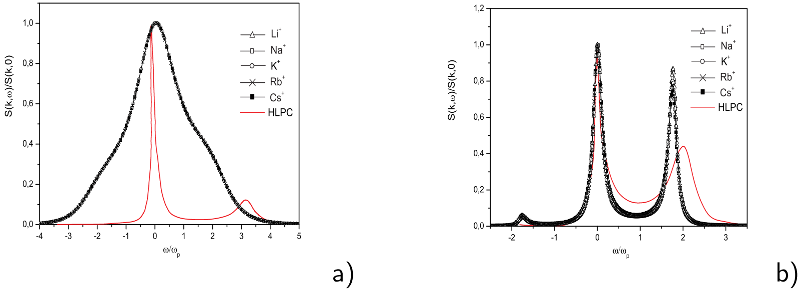


Figure: The relative charge-charge DSFs of alkali plasmas described above but at $k = 1.534/r_{ee}$, (a) $\Gamma_{ii} = 0.5$, (b) $\Gamma_{ii} = 2$ [4].

Taking into account the ion structure I

In a frame of the Adamjan's et al. HLPC model [10] one can include the ion structure through the function defining the fourth moment:

$$Q^{HGK}(k) = K(k) + L^{HGK}(k) + H^{HGK}. \qquad (26)$$

Here, the kinetic distribution is taken the same as in (18). We approximate here the contribution due to the electron-ion HGK correlations by the following expression:

$$H^{HGK} = \frac{h_{ei}(r=0)}{3} = \frac{g_{ei}(r=0)-1}{3} \simeq -\frac{1}{3}. \qquad (27)$$

The contribution $L^{HGK}(k)$ takes into account the electronic correlations, we calculated it for the HGK potential:

$$L^{HGK}(k) = \frac{1}{2\pi^2 n_e}\int_0^\infty p^2[S_{ee}(p)-1]f^{HGK}(p,k)dp, \qquad (28)$$

where

Taking into account the ion structure II

$$f^{HGK}(p,k) = \int_{-1}^{1} \frac{(ps-k)^2}{p^2-2psk+k^2}\zeta_{ee}(\sqrt{p^2-2pks+k^2})\frac{ds}{2} - \frac{\zeta_{ee}(p)}{3} \quad (29)$$

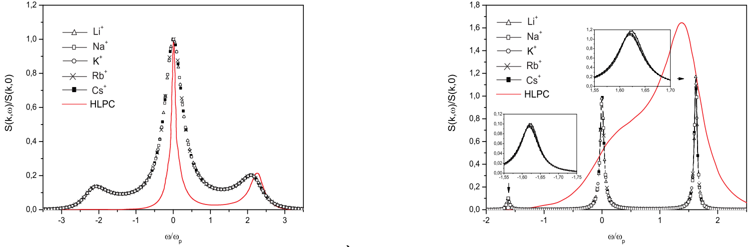
where $\zeta_{ee}(p)$ is to be determined from the Deutsch potential $\varphi_{ee}(p) = \Phi(p)\zeta_{ee}(p)$, where $\Phi(p) = 4\pi e^2/4\pi\varepsilon_0 p^2$ - Fourier transform of the Coulomb potential.

The equations (22-24) and ${\omega_1}^2$ in the equation (25) remain the same.

But the ${\omega_2}^2$ will turn into :

$${\omega_2}^2 = C_4/C_2 = {\omega_p}^2[1+K(k)+L^{HGK}(k)+H^{HGK}]. \quad (30)$$

Taking into account the ion structure III



a) b)

Figure: The relative charge-charge DSFs of alkali plasmas determined within HLPC model with the HGK static characteristics in comparison with the results of [10] obtained within the same HLPC model but with the Coulomb static characteristics at $k = 1.074 \cdot r_{ee}$. (a) $\Gamma_{ii} = 0.5$, Present results: $T = 30000K$, $n_e = 1.741 \cdot 10^{20} cm^{-3}$, Adamjan et al.: $T = 1574573K$, $n_e = 2.5 \cdot 10^{25} cm^{-3}$ and (b) $\Gamma_{ii} = 2$, Present results: $T = 30000K$, $n_e = 1.11 \cdot 10^{22} cm^{-3}$, S. V.

Taking into account the ion structure IV

Adamjan et al.: $T = 157457K$, $n_e = 1.61 \cdot 10^{24} cm^{-3}$, where the H, L are defined as (19) and (20), (21).

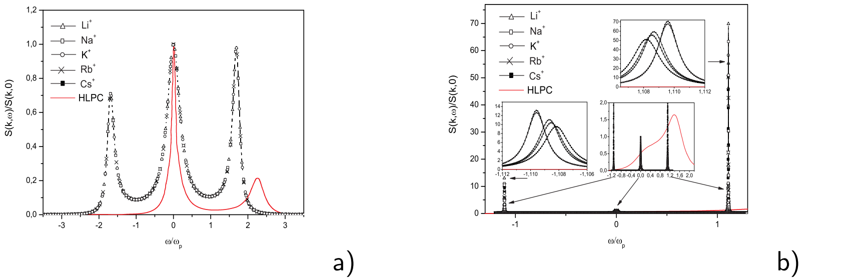


Figure: The relative charge-charge DSFs of alkali plasmas determined within HGK model with the HGK static characteristics in comparison with the results of [10] obtained within the same HLPC model but with the Coulomb static characteristics at $k = 1.074 \cdot r_{ee}$. (a) $\Gamma_{ii} = 0.5$, Present results: $T = 30000K$,

Taking into account the ion structure V

$n_e = 1.741 \cdot 10^{20} cm^{-3}$, Adamjan et al.: $T = 1574573K$, $n_e = 2.5 \cdot 10^{25} cm^{-3}$ and (b) $\Gamma_{ii} = 2$, Present results: $T = 30000K$, $n_e = 1.11 \cdot 10^{22} cm^{-3}$,S. V. Adamjan et al.: $T = 157457K$, $n_e = 1.61 \cdot 10^{24} cm^{-3}$, where the H^{HGK}, L^{HGK} are defined as (27) and (28), (29)

Conclusion I

- The partial and charge-charge SSFs have been calculated for alkali and Be^{2+} plasmas using the method described and discussed by Gregori et al. 2006, 2007. The DSFs for alkali plasmas have been calculated using the moment approach developed by V. M. Adamjan et al.1983, S. V. Adamjan et al. 1993.
- In both methods the screened Hellmann-Gurskii-Krasko pseudopotential with the soft ion core, obtained on the basis of Bogoljubov's method, taking into account not only the quantum-mechanical but also the repulsion due to the Pauli exclusion principle has been used.
- DSFs have been calculated within the HLPC and HGK model. The HLPC model was treated within the HGK model through the fourth moment of the loss function and with the static characteristics also determined for the screened HGK model. The results were compared to those of Adamjan et al. 1993 found within the HLPC model as well but with the pure Coulomb static characteristics.

Conclusion II

- We have detected deviations (in the values of the SSFs) from results obtained by Gregori et al. while we have noticed that the present dynamic results are in a reasonable agreement with those of Adamjan et al.: at higher values of k and with increasing k the curves damp while at lower values of k, and especially at higher Γ_{ee}, we observe sharp peaks also reported by Adamjan et al. At lower Γ_{ee} the curves for Li^+, Na^+, K^+, Rb^+ and Cs^+ do not differ while at higher Γ_{ee} the curves split. In alkali plasmas the plasmon peaks are more pronounced especially at higher Γ_{ii} and shifted in the direction of lower ω/ω_p than those considered within the Coulomb HLPC model with the Coulomb static characteristics. As the number of shell electrons increases 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 structure which we took into account by the HGK model compared to the HLPC model.

References

- J. P. Hansen and I.R. McDonald, Phys. Rev. A, **23**, 2041 (1981).
- , N.N. Bogoljubov *Studies in Statistical Mechanics*, (North-Holland 1962)
- S. Sadykova, W. Ebeling, I. Valuev and I. Sokolov, Contrib. Plasma Phys. **49**, 76-89 (2009).
- S. Sadykova, W. Ebeling, I. M. Tkachenko, Eur. Phys. J. D., DOI:10.1140/epjd/e2010-10118-y (2010)
- P. Seuferling, J. Vogel, C. Toepffer, Phys. Rev. A. 40, 323 (1989)
- G. Gregori, O.L. Landen, S.H., Glenzer, Phys. Rev. E 74, 026402 (2006)
- G. Gregori, A. Ravasio, A. Höll, S.H., Glenzer, S. J. Rose, High Energy Phys. 3, 99 (2007)
- V. M., Adamyan and I. M., Tkachenko, High Temp. (USA) 21, 307 1983.
- V. M., Adamyan, T. Meyer, and I. M., Tkachenko, Sov. J.Plasma