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Yu.V. Arkhipov[1], A.B. Ashikbaeva[1], A. Askaruly[1*], V.V. Voronkov[1], A.E. Davletov[1],
D. Dubovtsev[1], K.V. Starikov and I.M. Tkachenko[2]
[1]Scientific-Research Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, Kazakhstan,
[2]Instituto de MatemáticaPura y Aplicada, Universidad Politécnica de Valencia, Spain

Static properties of plasmas modeled by the kelbg pseudopotential

Abstract. The partial radial distribution functions and static structure factors of hydrogen-like two component plasmas modeled with the Kelbg pseudopotential are calculated within the Ornstein-Zernike approximation. It is shown that the simulation data on the inverse dielectric function satisfies five convergent sum rules and other exact relations. The sum rules which are the power frequency moments of the loss function, which determines the polarizational stopping power of a plasma characterized by the inverse dielectric function are computed using the Kelbg potential. Results on long-wavelength values of the loss function power moments calculated from the simulation data in comparison to the exact values are presented.

Keywords: Kelbg pseudopotential, Ornstein-Zernike approximation, radial correlation functions, static structure factors, sum rules, method of moments.

To study the dynamic structural properties of dense nonideal plasma for example by the method of moments it is necessary to solve the problem of obtaining the static structure factors and the radial distribution functions [1]. The values of these static functions can be obtained from experimental data, Monte Carlo, molecular dynamics [2], and with the help of numerical calculations by solving the Ornstein-Zernike equation in the HNC approximation [3].

In the first part of the work we present the modified Kelbg pseudopotential, which were obtained in [4].

In the second part we present our results on static structure factors and the radial distribution functions calculated within the Kelbg pseudopotential

And at last part we state our last results on static dielectric function.

For Hydrogen-like plasmas when $n_e = Zn_i$ the corrected Kelbg pseudopotential, which reproduces the equilibrium properties of the quantum Coulomb system via classical statistics, has the following form

$$\phi_{ab}^{K}(r) = \phi_{ab}^{K1}(r) - \phi_{ab}^{K2}(r), \qquad (1)$$

where

$$\phi_{ab}^{K1}(r) = \frac{Z_a Z_b e^2}{r} F\left(\frac{r}{\lambda_{ab}}\right) = \frac{Z_a Z_b e^2}{\lambda_{ab} x_{ab}} F(x_{ab}),$$

$$\phi_{ab}^{K2}(r) = A_{ab}(\xi_{ab}) \beta^{-1} \exp\left(-x_{ab}^2\right),$$

with wavelength

$$\lambda_{ab} = \hbar \sqrt{\frac{\beta}{2m_{ab}}}, \quad \xi_{ab} = -\frac{Z_a Z_b e^2 \beta}{\lambda_{ab}},$$

reduced mass

$$m_{ab} = \frac{m_a m_b}{m_a + m_b}, \quad x_{ab} = \frac{r}{\lambda_{ab}},$$

and

$$F(x) = 1 - \exp\left(-x^2\right) + \sqrt{\pi} x \left(1 - \operatorname{erf}(x)\right),$$

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-s^2\right) ds,$$

$$A_{ee}(\xi_{ee}) = \sqrt{\pi} |\xi_{ee}| + \ln\left(2\sqrt{\pi} |\xi_{ee}| G\left(|\xi_{ee}|\right)\right),$$

$$G(\xi) = \int_0^\infty \frac{y \exp\left(-y^2\right) dy}{\exp(\pi\xi / y) - 1}, \quad \zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}.$$

$$A_{ei}(\xi_{ei}) = -\sqrt{\pi}\xi_{ee} + \ln\Big(\left(\sqrt{\pi}\xi_{ei}^3 \left(\zeta(3) + \zeta(5)\xi_{ei}^2 / 4\right)\right) - 4\sqrt{\pi}\xi_{ei} G(\xi_{ei})\Big),$$

$\zeta(n)$ is the Riemann-Zeta function.

The Fourier transform of the modified Kelbg potential:

[*] Corresponding author e-mail: adilask@gmail.com

$$\phi_{ab}^{K}(k)=\frac{8\pi Z_a Z_b e^2}{k^3\lambda_{ab}}D\left(\left(\frac{k\lambda_{ab}}{2}\right)\right)-A_{ab}(\xi_{ab})\beta^{-1}\pi^{3/2}\lambda_{ab}^3\exp\left(-\frac{(k\lambda_{ab})^2}{4}\right),$$

where

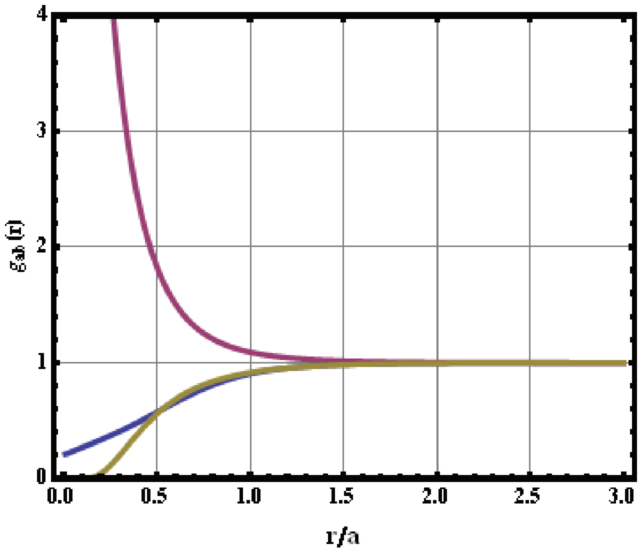
$$D(s)=\exp(-s^2)\int_0^s\exp(t^2)\,dt$$

is the Dawson integral. Notice that in the classical limiting case,

$$\phi_{ab}^{K}(k\to 0)\simeq\frac{4\pi Z_a Z_b e^2}{k^2}.$$

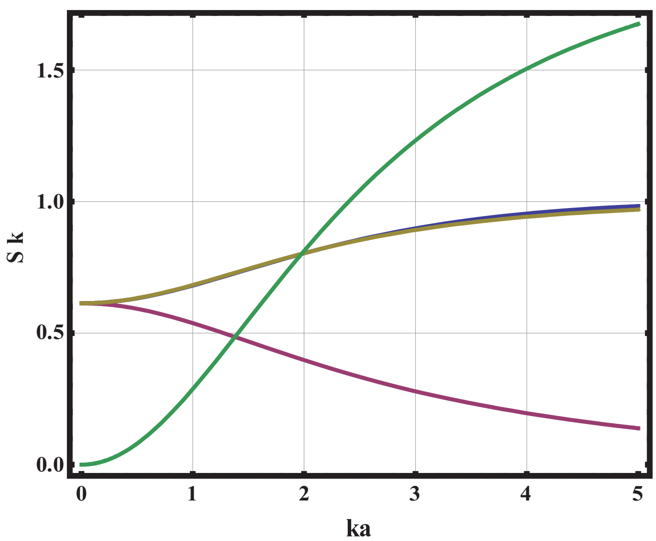
On the basis of the mentioned Kelbg pseudopotential (eq. 1) we made calculations of the radial correlation functions (Fig. 1) and the static structure factors (Fig. 2) through the HNC approximation scheme where the SSF of charge-charge interaction

$$S_{cc}(k)=S_{ee}(k)+S_{ii}(k)-2S_{ei}(k).$$



Blue line – electron-electron interaction
Brown line –ion-ion interaction
Red line – electron-ion interaction

Figure 1 - Radial distribution function at $T=100000K,\ n_e=5.1324\times10^{22}cm^{-3}$ $(\Gamma=1,\, r_s=3.15448,\, \theta=1.7111)$.



Blue line – electron-electron interaction
Brown line –ion-ion interaction
Red line – electron-ion interaction
Green line – charge-charge interaction

Figure 2 - Partial static structure factors at same conditions.

The sum rules are the power moments: of the loss function

$$\mathrm{L}(k,\omega) = -\frac{\mathrm{Im}(\varepsilon^{-1}(k,\omega)}{\omega},$$

which determines the polarizational stopping power of a plasma characterized by the inverse dielectric function, a genuine response function, $\varepsilon^{-1}(k,\omega)$ [4]:

$$C_l(k) = \pi^{-1}\int_{-\infty}^{\infty}\omega^l \mathrm{L}(k,\omega)d\omega\,,\quad l = 0,1,2,3,4,$$

$$C_0(k) = 1-\varepsilon^{-1}(k,0)\,,\quad C_1(k) = C_3(k) = 0\,,\quad C_2(k) = \omega_p^2\,,$$

For different types of plasma there are different view of the fourth moment

$$\frac{C_4(k)}{\omega_p^4} = \begin{cases} 1+V(k)+U(k), & \text{OCP} \\ 1+V(k)+U(k)+H, & \text{TCP} \\ \zeta_{ee}(k)+V(k)+U(k)+H, & \text{model TCP} \end{cases}$$

In general case

$$C_4(k) = \omega_p^4\left(\zeta_{ee}(k)+V(k)+U(k)+H\right),$$

where

$$\phi_{ab}(k) = \left(4\pi e^2/k^2\right)\zeta_{ab}(k)\,,\quad a,b = e,i,$$

The kinetic part is determined as

$$V(k) = \frac{\langle v_e^2\rangle k^2}{\omega_p^2}+\left(\frac{\hbar}{2m}\right)^2\frac{k^4}{\omega_p^2},$$

where $\langle v_e^2\rangle$ is the average of the square of the (electron) velocity, and

$$U(k) = \frac{1}{2\pi^2 n_e}\int_0^{\infty} q^2\left(S_{ee}(q)-1\right)\left(\frac{Z_{ee}(q)}{8}-\frac{\zeta_{ee}(q)}{3}\right)dp\,,$$

$$Z_{ab}(q) = \int_{q-k}^{q+k}\zeta_{ab}(p)\left(q^2-k^2-p^2\right)^2\frac{dp}{qk^3p},$$

$$H = \frac{1}{6\pi^2 n_e\sqrt{Z}}\int_0^{\infty} q^2 S_{ei}(q)|\zeta_{ei}(q)|dp\,,$$

while, in a Coulomb hydrogen plasma,

$$H_C = h_{ei}(0)/3.$$

The loss function is an even function of frequency so that we deal with two sets of moments: $\{C_0,0,C_2\}$ and $\{C_0,0,C_2,0,C_4\}$. In TCPs $C_6 = \infty$, but in OCP higher order moments usually converge.

The formfactor

$$\zeta_{ab}(k) = \frac{\phi_{ab}^K(k)k^2}{4\pi e^2} = \frac{2Z_aZ_b}{k\lambda_{ab}}D\left(\left(\frac{k\lambda_{ab}}{2}\right)\right)-\frac{A_{ab}(\xi_{ab})\sqrt{\pi}}{4e^2\beta}k^2\lambda_{ab}^3\exp\left(-\frac{(k\lambda_{ab})^2}{4}\right),$$

recovers the value Z_aZ_b in the $k\to 0$ limit. This implies that the characteristic frequency

$$\omega_2^2 = \frac{C_4(k)}{\omega_p^2} = \omega_p^2\left(\zeta_{ee}(k)+V(k)+U(k)+H\right)$$

in the long-wavelength limiting case [4] tends to the plasma frequency squared multiplied by (1+H).

The static dielectric function was approximated as

$$\varepsilon^{-1}_{classical}\left(k,0\right)=1-\frac{4\pi e^2\beta\sqrt{n_e n_i}}{k^2}\left[S_{ee}\left(k\right)+S_{ii}(k)+S_{ei}(k)\right].$$

Results on long-wavelength values of the loss function power moments calculated from the data of [4] in comparison to the exact values are presented in Table 1.

Table 1 – Long-wavelength values of the loss function power moments

	$T=100000K$, $n_e=5.1324\times10^{22}cm^{-3}$	$T=64000K$, $n_e=1.3454\times10^{22}cm^{-3}$
C_0	1	1
$C_2(k)/\omega_p^2$	1	1
$C_4(k)/\omega_p^4$	2.00689	2.72547
$1+H$	2.01315	2.73321

Conclusion

The radial distribution function and the static structure factor in the HNC approximation for the two component plasma were obtained on the basis of modified Kelbg interaction pseudopotential. With the help of these static characteristics the moments of the loss function were calculated and tested on the satisfiability of sum rules.

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