*36th EPS Conference on Plasma Phys. Sofia, June 29 - July 3, 2009 ECA Vol.**33E**, P-5.076 (2009)*

Electric Microfield Distributions (EMD) in Alkali Plasmas with Account of the Ion Structure in a Moderately Coupled Approximation

S.P. Sadykova*[1], W. Ebeling[1], I. Valuev[2], I. M. Sokolov[1]

[1] *Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany*

[2] *Joint Institute for High Temperatures of RAS, Izhorskaya, 13, bld. 2, Moscow 125412, Russia*

Pseudopotentials taking into account the ion structure. Hellmann-Gurskii-Krasko potential. Screening of the Hellmann-Gurskii-Krasko potential

High-temperatures alkali plasmas are widely applied in many technical projects [1]. For the calculations of the EMD at a charged particle we need as an essential input quantity the pair distribution functions determined by the effective interactions of the plasma particles [2], [1]. In particular, the Deutsch [3] and the corrected Kelbg [4] are frequently used. In the present work we use only the electron-electon part of the corrected Kelbg potential:

$$\varphi_{ee}(r) = \frac{e^2}{4\pi\varepsilon_0}\left\{\frac{1-e^{-r^2/\lambda_{ee}^2}}{r} + \frac{\sqrt{\pi}}{\lambda_{ee}}(1-erf(r/\lambda_{ee}))\right\} - k_BT\tilde{A}_{ee}(\xi_{ee})\exp(-(r/\lambda_{ee})^2) \tag{1}$$

with $\tilde{A}_{ee} = \sqrt{\pi}\,|\xi_{ee}| + \ln\left[2\sqrt{\pi}\,|\xi_{ee}|\int\limits_0^\infty dyy\exp(-y^2)/(\exp(\pi\,|\xi_{ee}|/y)-1)\right]$, where $\lambda_{ee} = \hbar/\sqrt{m_e k_B T}$ is De Broglie wave length of relative motion, here m_e is the electron mass, $\hbar$ is the Planck constant and k_B is the Boltzmann constant. Here $\varsigma(x)$ denotes Riemann's Zeta-function and $\xi_{ee} = -(e^2)/(4\pi\varepsilon_0 k_B T\lambda_{ee})$ is the interaction parameter. These models are valid for high temperature plasmas when the ions are bare or there is no significant influence of the ion shell structure. In order to correctly describe alkali plasmas at moderate temperatures one needs to take into account the ion structure. In the previous works [1], [5] we described the electron-ion and ion-ion Hellmann-Gurskii-Krasko (HGK) potentials [6] which takes into account the ion structure shown in the Figures 1a and 2a:

$$\varphi^{HGK}{}_{ab}(r) = \frac{e_a e_b}{4\pi\varepsilon_0}\frac{1-e^{-r/R_{Cab}}}{r} + \frac{|e_a e_b|}{4\pi\varepsilon_0}\frac{a}{R_{Cab}}e^{-r/R_{Cab}}, \tag{2}$$

where $a,b = i,e,\ e_e = e,\ e_i = ze$ are electric charges, with $z-$ valency, $R_C = r_C r_B$ $(R_{Cii} = 2R_{Cei})$ and a [6] are determined experimentally using the ionisation potential and the formfactor of the screened pseudopotential at the first sites of the reciprocal lattice. It is of a high interest to construct the pseudopotential model which takes into account not only the quantum-mechanical and the ion shell structure but also the screening field effects. In order to include the screening effects, in [1] we applied the method developed in [7] which is based on the chain of Bogoljubow equations [8]. Here as micropotentials we use the $e-i$, $i-i$ HGK pseudopotentials (2) and $e-e$ corrected Kelbg potential (1) instead of the earlier employed Deutsch potential [3]. The motivation for doing so is that the corrected Kelbg potential provides better results at the low temperatures when quantum effects start to play a significant role. For this purpose we solve in Fourier space the following system of linear algebraic equations:

$$\Phi_{ab}(k) = \varphi_{ab}(k) - \frac{1}{k_BT}\left[n_e\varphi_{ae}(k)\Phi_{eb}(k) + n_i\varphi_{ai}(k)\Phi_{ib}(k)\right] \tag{3}$$

where $a,b = i,e$, $\varphi_{ab}(k)$ are the Fourier transforms of (1)- (2). The solution of the system (3) reads:

$$\Phi_{ei}(k) = \frac{Ze^2}{\varepsilon_0\Delta}\frac{(2a-1){R_{cei}}^2k^2-1}{k^2(1+k^2{R_{cei}}^2)^2}, \tag{4}$$

$$\Phi_{ee}(k) = \frac{e^2}{\varepsilon_0\Delta}\left\{\frac{2\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)}{k^3\lambda_{ee}}\int_0^{k\lambda_{ee}/2}e^{t^2}dt+\right. \tag{5}$$

*Corresponding author: e-mail: saltanat@physik.hu-berlin.de

$$\frac{1}{k^4 r_{Di}^2}\left[\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\frac{2((2a+1)R_{cii}{}^2k^2+1)}{k\lambda_{ee}(1+k^2R_{cii}{}^2)^2}\int_0^{k\lambda_{ee}/2}e^{t^2}dt-\left(\frac{(2a-1)R_{cei}{}^2k^2-1}{(1+k^2R_{cei}{}^2)^2}\right)^2\right]-$$
$$A\tilde{A}_{ee}(\xi_{ee})\left(1+\frac{(2a+1)R_{cii}{}^2k^2+1}{k^2r_{Di}{}^2(1+k^2R_{cii}{}^2)^2}\right)\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\Bigg\},$$

$$\Phi_{ii}(k)=\frac{Z^2e^2}{\varepsilon_0\Delta}\left\{\frac{(2a+1)R_{cii}{}^2k^2+1}{k^2(1+k^2R_{cii}{}^2)^2}+\right. \tag{6}$$
$$\frac{1}{k^4 r_{De}^2}\left[\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\frac{2((2a+1)R_{cii}{}^2k^2+1)}{k\lambda_{ee}(1+k^2R_{cii}{}^2)^2}\int_0^{k\lambda_{ee}/2}e^{t^2}dt-\left(\frac{(2a-1)R_{cei}{}^2k^2-1}{(1+k^2R_{cei}{}^2)^2}\right)^2\right]-$$
$$\left.A\tilde{A}_{ee}(\xi_{ee})\frac{(2a+1)R_{cii}{}^2k^2+1}{k^2r_{De}{}^2(1+k^2R_{cii}{}^2)^2}\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\right\},$$

here r_{De}, r_{Di} are the Debye radius of electrons and ions respectively, where $1/r_{Di}{}^2 = z^2e^2n_i/(\varepsilon_0 k_BT)$, $1/r_{De}{}^2 = e^2n_e/(\varepsilon_0 k_BT)$, $A = k_BT\pi^{3/2}\lambda_{ee}^3\varepsilon_0/e^2$ and Δ is:

$$\Delta = 1+\frac{2\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)}{k^3r_{De}{}^2\lambda_{ee}}\int_0^{k\lambda_{ee}/2}e^{t^2}dt+\frac{(2a+1)R_{cii}{}^2k^2+1}{k^2r_{Di}{}^2(1+k^2R_{cii}{}^2)^2}+ \tag{7}$$
$$\frac{1}{k^4 r_{De}{}^2r_{Di}{}^2}\left[\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\frac{2((2a+1)R_{cii}{}^2k^2+1)}{k\lambda_{ee}(1+k^2R_{cii}{}^2)^2}\int_0^{k\lambda_{ee}/2}e^{t^2}dt-\left(\frac{(2a-1)R_{cei}{}^2k^2-1}{(1+k^2R_{cei}{}^2)^2}\right)^2\right]-$$
$$\frac{A\tilde{A}_{ee}(\xi_{ee})}{r_{De}{}^2}\left(1+\frac{(2a+1)R_{cii}{}^2k^2+1}{k^2r_{Di}{}^2(1+k^2R_{cii}{}^2)^2}\right)\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right),$$

The present approximation is restricted to the constraint $\Gamma \lesssim 1$. The pseudopotential $\Phi_{ab}(r)$ can be restored from (4-7) by Fourier transformation

$$\Phi_{ab}(r)=\frac{1}{2\pi^2 r}\int\Phi_{ab}(k)k\sin(kr)dk \tag{8}$$

In a weakly coupled regime the equation (5) turns into the following

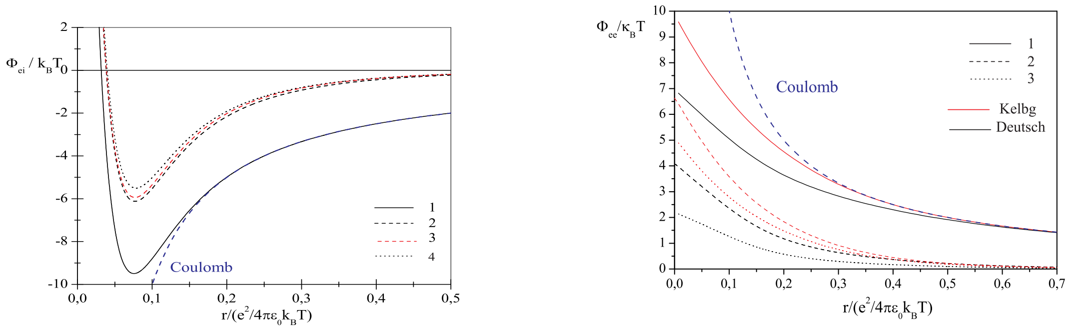
$$\varphi_{ee}(r)=\frac{e^2}{4\pi\varepsilon_0}\left\{\frac{e^{-r/r_D}-e^{-r^2/\lambda_{ee}^2}}{r}+\frac{\sqrt{\pi}}{\lambda_{ee}}(1-erf(r/\lambda_{ee}))\right\}-k_BT\tilde{A}_{ee}(\xi_{ee})\exp(-(r/\lambda_{ee})^2) \tag{9}$$

with $\frac{1}{r_D{}^2}=\sum_{c=e,i}\frac{e_c{}^2n_c}{\varepsilon_0 k_BT}$. As one can clearly see from the Figures 1a, b and 2a at large $\Gamma = e^2/(4\pi\varepsilon_0 r_{ee})$ ($r_{ee} = (3/(4\pi n_e))^{1/3}$ is the $e-e$ interparticle distance) the difference between the screened HGK potentials (4-7) and corresponding unscreened potentials (7) in [1], (1) and (2) is quite large, whereas when Γ decreases the difference becomes not so much considerable. In a case for $e-e$ interaction at relatively low temperature $T = 8000K$ and small distances the difference between the corrected Kelbg and the Deutsch potentials as well as between them and their corresponding screened potentials is significant. This can be explained by that fact that, as mentioned earlier, at low temperatures and high densities (Γ) the screening and quantum effects start to play a big role. It is worth to note that the Debye approximation of the potentials (9) and (20), (21) in [1] describes quite well behaviour of the screened HGK potential at small Γ as shown in Fig. 2b. However, at the large value of Γ one can observe small discrepancy between this potential and the screened HGK potential at the small distances $R = r/r_L$.

Electric Microfield Distributions at the location of an ion with the account of ion structure

We consider the two-component electron-ion Li^+, Na^+, K^+, Cs^+ thermally equillibrium and isotropic plasma ($Ze_- = -e_+$ (Z=1) and masses $m_i >> m_e$) consisting of $N = N_e + N_i + N_R$ ($N_e = N_i, N_R = 1$) charged particles and a radiator (ion) at a temperature T in a volume Ω. The method which is used for the calculation is the coupling-parameter integration technique for two-component plasmas introduced by Ortner et al. [2]. The final calculation formular for the microfield probability distribution function at an ion is the following

$$P(\beta)=\frac{2\beta}{\pi}\int_0^\infty l^*T_i(l^*)\sin(\beta l^*)dl^* \tag{10}$$



a) b)

Figure 1: Comparison between the different $e-i$ **(a)** and $e-e$ **(b)** pseudopotentials of Cs^+ plasma against the dimensionless distance $R = r/r_L$, here $r_L = e^2/(4\pi\varepsilon_0 k_B T)$ at $\Gamma \approx 1.56$, $T = 8000K, n_e = 10^{26} m^{-3}$. **(a)** 1: HGK potential (2); 2: Screened HGK potential with the Deutsch potential as micropotential (11) in [1]; 3: Screened HGK potential (4) with the corrected Kelbg potential (1) as micropotential; 4: $e-i$ Screened HGK potential in the Debye approximation (20) in [1]; **(b)** The corrected Kelbg (red) and Deutsch (black) sets of potentias. 1: Corrected Kelbg (1) or Deutsch potential (7) in [1]; 2: Screened HGK potential with the corrected Kelbg (5) or Deutsch potentials as micropotentials (12) in [1]; 3: $e-e$ Screened HGK potential in the Debye approximation with Deutsch (21) in [1] or corrected Kelbg potentials (9) as mictopotentials.

Here $T(l)$ is the Fourier transform of the electric microfield distribution $Q =< \exp(\imath\vec{k}\cdot\vec{E}) >$ with $\vec{E}$ being the total electric microfield, $\beta = \varepsilon/\varepsilon_0$, $l^* = l\varepsilon_0$, $\varepsilon_0 = e/(4\pi\varepsilon_0 r_{ei}^2) = en^{2/3}/((36\pi)^{1/3}\varepsilon_0)$ with $r_{ei} = (3/(4\pi n))^{1/3}$ being the $e-i$ interparticle distance, where $n = N/\Omega$, $n = n_e + n_i$. Assuming that our system is isotropic we used the relation $4\pi Q(\vec{\varepsilon})\varepsilon^2 d\varepsilon = P(\varepsilon)d\varepsilon$. The parameters T, Γ are beyond the degeneration border ($n_e \cdot \lambda_{ee}^3 < 1$) and can be treated classically ($r_L/\lambda_{ee} > 1$). The main result of the method [2] for TCP case in the Debye approximation is the following:

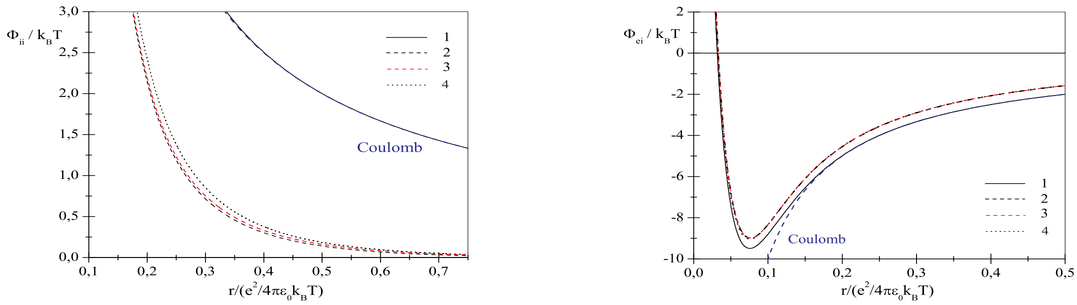
$$\ln T_i(l) = \frac{n}{2} e \int_0^l d\lambda \int_0^\infty d\vec{r}\phi(\vec{r})\,[g_{ii}(\vec{r},\lambda) - g_{ie}(\vec{r},\lambda)], \tag{11}$$

where $\phi(r) = -i\hat{l}\cdot\vec{\nabla}V$, where $V(r) = e/(4\pi\varepsilon_0 r)$ is the Coulomb potential, $\hat{l}$ - a unit vector of $\vec{l}$ and $g(\vec{r},\lambda)$ is the two-body correlation function with the "coupling strength" (charging) parameter $0 \le \lambda \le 1$:

$$g_{ia}(\vec{r};\lambda) \cong g_{ia}(\vec{r},0)\exp\left\{-i\lambda\hat{l}\cdot\vec{\nabla}_0 \frac{e_a}{4\pi\varepsilon_0 k_B T r}\exp(-r/r_D)\right\}, \tag{12}$$

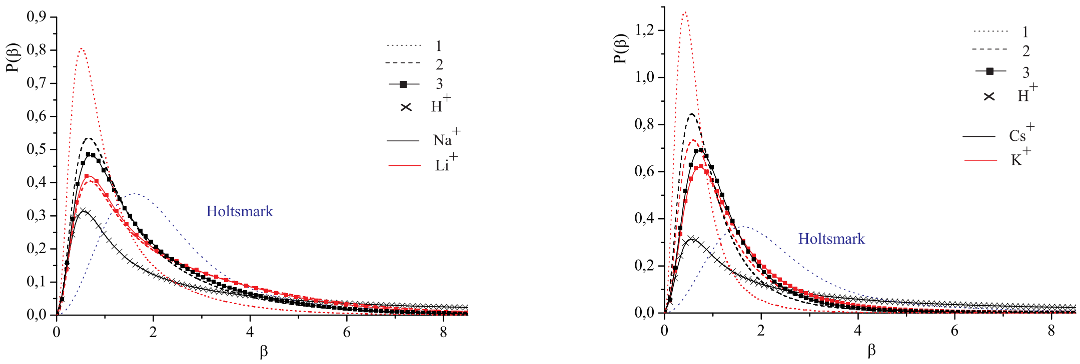
$$g_{ia}(r,0) = \exp\left(-\Phi_{ia}(r)/k_B T\right). \tag{13}$$

Here $g_{ia}(\vec{r},0)$ is the normal pair distribution function or (RDF) of the pair i,a given by the screened potentials (4-6) as described in the previous section or (11-14) in [1] . In the recent work [5] on a base of the Ortner method the EMD for alkali plasmas at low and moderately large Γ have been calculated. There the RDFs have been determined in the Debye approximation (20) in [1] (weakly coupled regime). Here we use a better approximation for RDF, namely the RDF in a moderately coupled approximation obtained with the help of the screened HGK (11 -14) in [1]. As one can see in the Fig. 3a, b, there is a good agreement between the EMD in the moderately coupled approximation and the Monte Carlo (MC) simulations, whereas there is a big discrepancy between the EMD in Deby approximation and MC. In a case of Li^+ the curves almost coinside. This can be explained by that fact that the screening effects in equations (11 -14) in [1] are better taken into account than in equations (9) and (20), (21) in [1] for a weakly coupled plasma. It is worth to note that with an increase of number of band electrons in a closed shell from Li^+ till Cs^+ the discrepancy between the present theory and MC grows. This demonstrates again the significant role of ion structure at large values of Γ. This allows us to conclude that the proposed approach makes



a) b)

Figure 2: Comparison between the different $i-i$ **(a)** and $e-i$ **(b)** pseudopotentials of Cs^+ plasma at $T = 8000K$, **(a)** $\Gamma \approx 1.56$, $n_e = 10^{26}m^{-3}$ and **(b)** $\Gamma \approx 0.335$, $n_e = 10^{24}m^{-3}$. **(a)** 1: HGK potential (2); 2: Screened HGK potential with the Deutsch potential as micropotential (13) in [1]; 3: Screened HGK potential (6) with the corrected Kelbg potential (1) as micropotential ; 4: $i-i$ Screened HGK in the Debye approximation (20) in [1]; **(b)** Description of the legend is the same as in the Fig. 1 (a).



a) b)

Figure 3: Comparison of EMD calculations in a frame of the Hellmann-Gurskii-Krasko pseudopotential model for H^+, **(a)** Li^+, Na^+ and **(b)** K^+, Cs^+ plasmas at $T = 30000K$ and $\Gamma = 2$. 1: EMD with RDF (13) obtained from the screened HGK in Debye approximation (20) in [1]; 2: EMD with RDF obtained from the screened HGK in the moderately coupled approximation (11-14) in [1]; 3: Monte Carlo simulations (MC).

a remarkable approvement in the EMD calculation at moderately large Γ and should be studied in a future.

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