Electric Microfield Distributions and their Tails with Account of the Ion Core Structure

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Plasma Parameters

$$r_{ab} = \left(\frac{3}{4\pi n_{a,b}} \right)^{1/3}, a,b = e,i$$ - **the mean distance between the particles**

$$r_L = \frac{e^2}{4\pi\varepsilon_0 k_B T}$$ - **Landau length**

$$\Gamma_{ab} = \frac{e^2}{4\pi\varepsilon_0 k_B T r_{ab}}, a,b = e,i$$ - **coupling parameter**

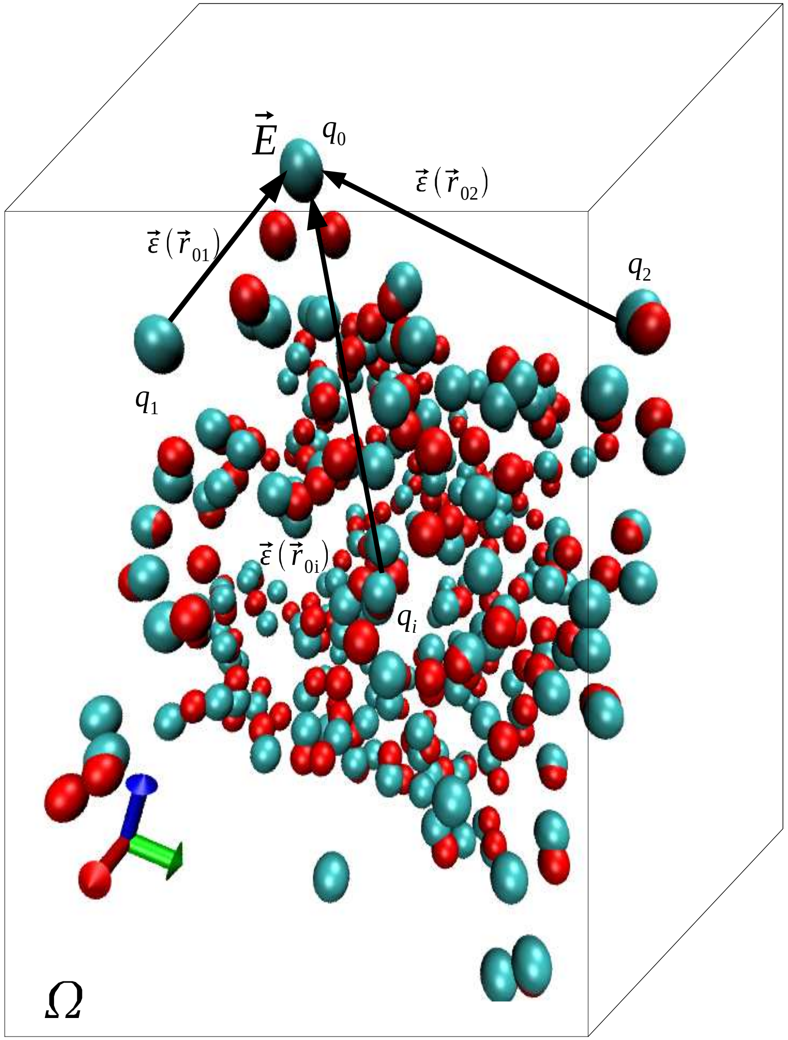
$$\Lambda_K = \frac{\hbar}{(m_K k_B T)^{1/2}}$$ - **thermal de-Broglie wavelength, where k =i, e**

$$\lambda_{ab} = \frac{\hbar}{\sqrt{2\pi\mu_{ab} k_B T}}$$ - **thermal de-Broglie wavelength for the relative motion of electrons and ions, where μ_{ab}- reduced mass of a-b pair**

$$\frac{\Lambda_e}{r_{ee}} > 1$$ - **degeneration region parameter**

$$\frac{r_L}{\Lambda_e} > 1$$ - **classical region parameter**

Definition of EMD



$$Q(\vec{\in}) = \lim_{\substack{N,\Omega\to\infty \\ N/\Omega=n}} Z^{-1}\int\ldots\int d\vec{r}_0 d\vec{r}_1\ldots d\vec{r}_N e^{\frac{-V}{k_B T}} \times \delta(\vec{\in} - \vec{E}),$$

where $\vec{E} = \sum_{j=1}^{N} \vec{\varepsilon}(\vec{r}_{0j}), \vec{\varepsilon}(\vec{r}_{0j}) = \frac{q_j}{r_{0j}^2}\hat{r}_{0j}$

Z- configurational partition function of N+1 particle system; $N=N_i+N_e$

V- potential energy of the system:

$$V = \sum_{0=i<j} \upsilon_{ij},\ \upsilon_{ij} = \frac{q_i q_j}{\vec{r}_{ij}}$$

$$P(\in) = 4\pi \in^2 Q(\in) = \frac{2\in}{\pi}\int_0^\infty lT(l)\sin(\in l)dl,$$

here $T(\vec{l}) = \int Q(\vec{\in}) e^{i\vec{l}\cdot\vec{\in}} d\vec{\in} = \left\langle e^{i\vec{l}\cdot\vec{E}} \right\rangle$

Pseudopotential Models.
Hellmann Potential

Hans G.A. Hellmann (1903-1938)

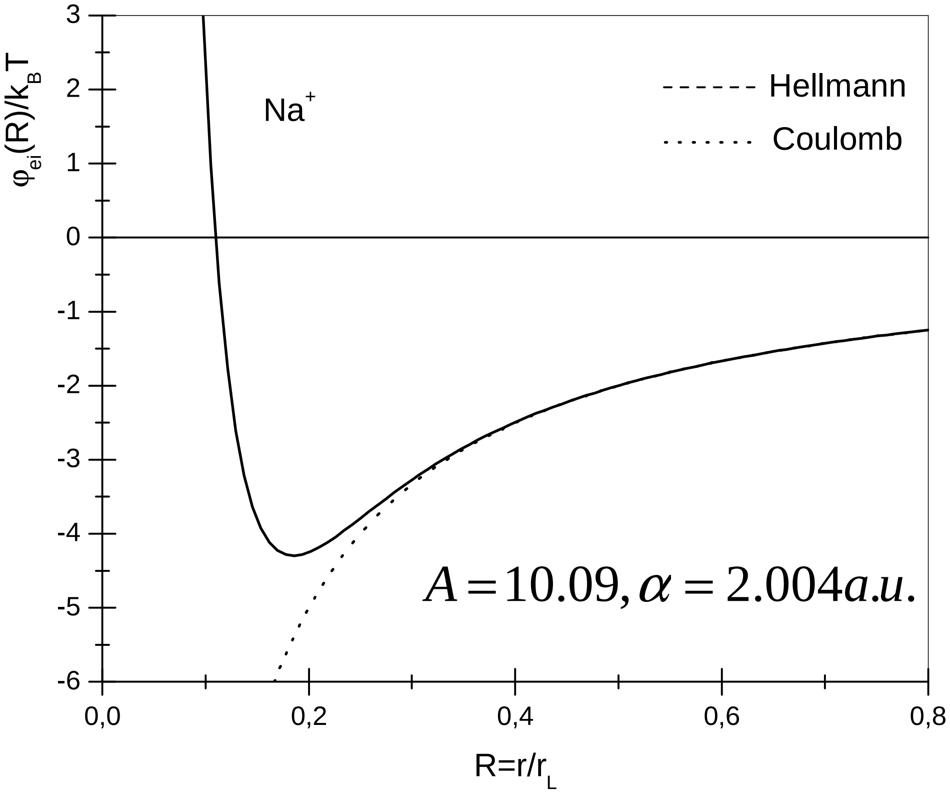
• Born on the 14th of October in Wilhelmshaven, Germany
• Sentenced to death on the 29th of May 1938

Fundamental Contributions:

• The molecular virial Hellmann-Slater theorem (1933)
• The Hellmann-Feynman (molecular force) theorem (1936)
• Pseudopotentials (1934)

Hans Hellmann in the 1930s

Pseudopotential or Effective Core Potential [1]



$$\varphi^{H}_{ei} = -\frac{ze^2}{4\pi\varepsilon_0 r} + \frac{e^2}{4\pi\varepsilon_0}\frac{Ae^{-\alpha r}}{r}$$

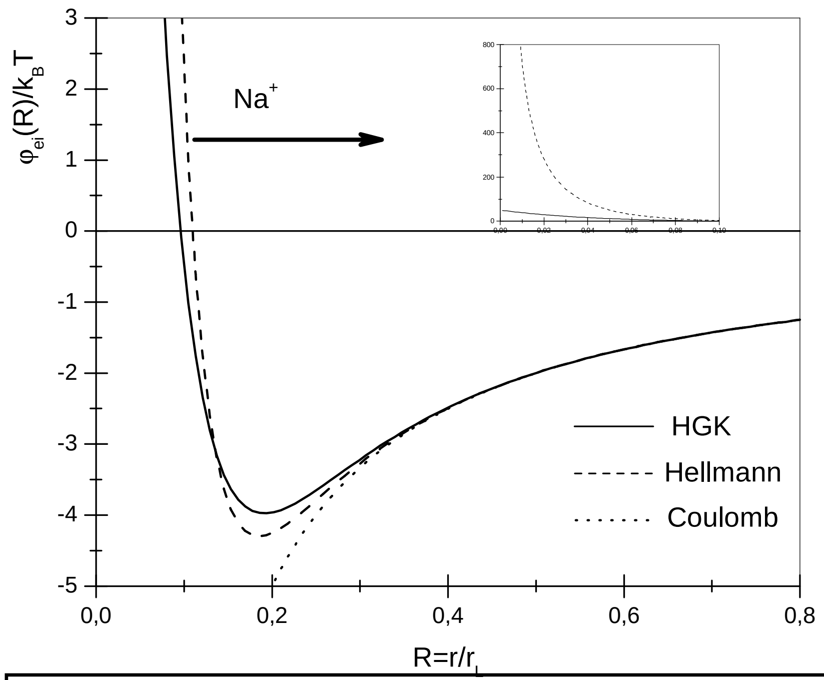
The repulsive „additional“ potential *as the result of the Pauli-principle*

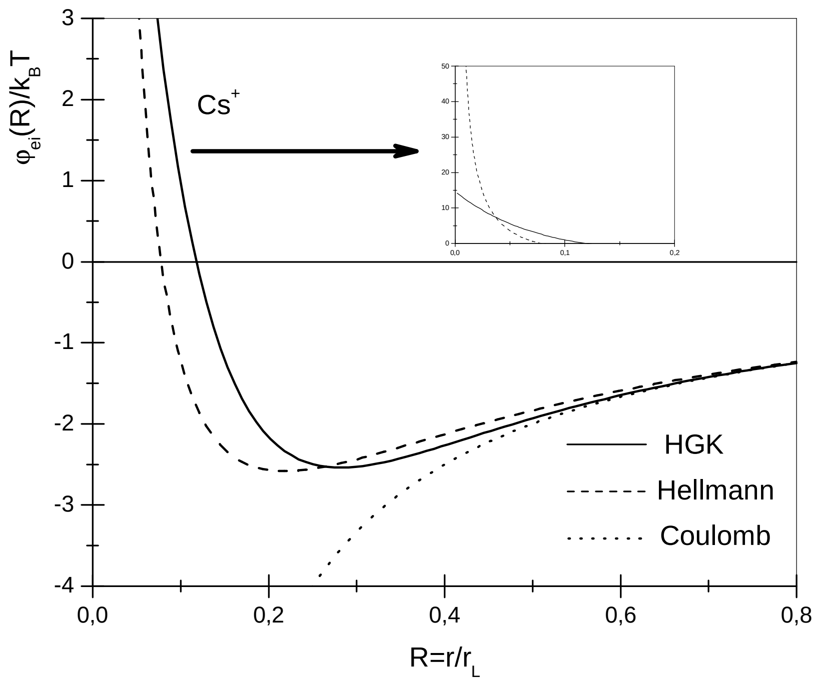
[1] *H. Hellmann, J. Chem. Phys.* ***3****, 61 (1935); Acta Fizicochem. USSR,* ***1****, 913 (1935);* ***4****, 225 (1936)*

Pseudopotential Models.

Hellmann-Gurskii-Krasko (HGK) Potential [2]

Electron-Ion Interaction





$$\varphi_{ei} = -\frac{ze^2}{4\pi\varepsilon_0}\frac{1-e^{-r/R_{Cei}}}{r} + \frac{ze^2}{4\pi\varepsilon_0}\frac{a}{R_{Cei}}e^{-r/R_{Cei}}$$

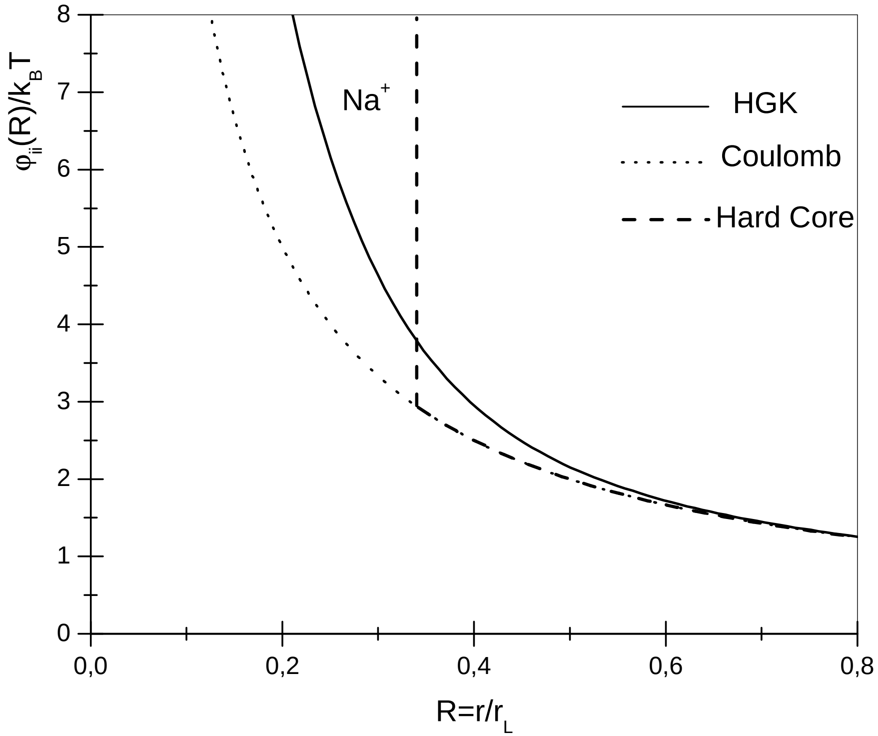
z- Valency, a, R_{Cei}- are adjustable to the optical spectra parameter

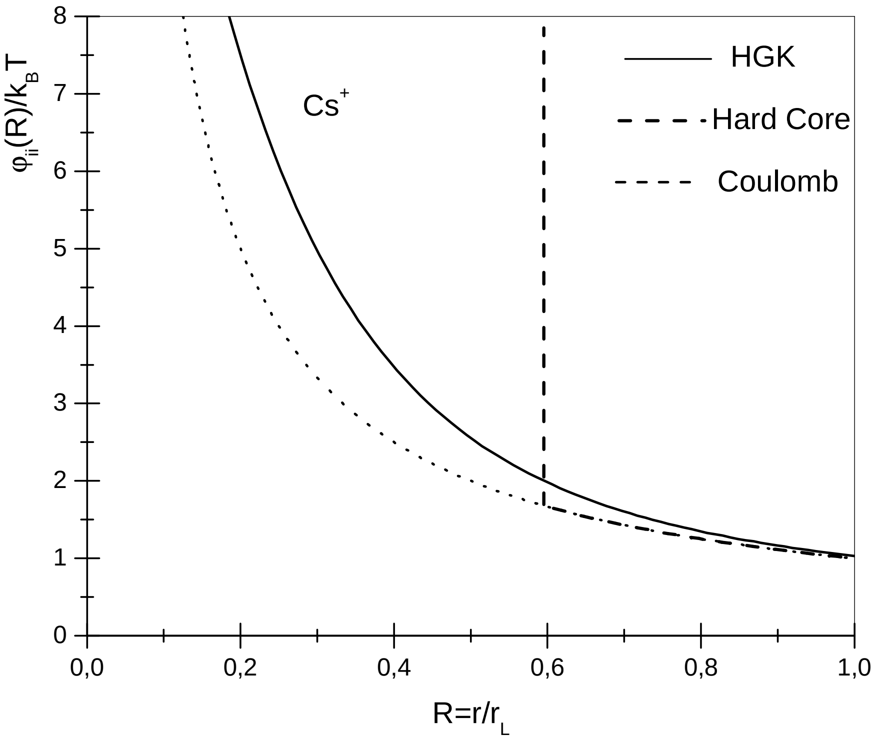
[2] *G. L.Krasko , Z. A. Gurskii, JETP letters* ***9****, 363 (1969).;*

Pseudopotential Models.

Hellmann-Gurskii-Krasko Potential

Ion-Ion Interaction

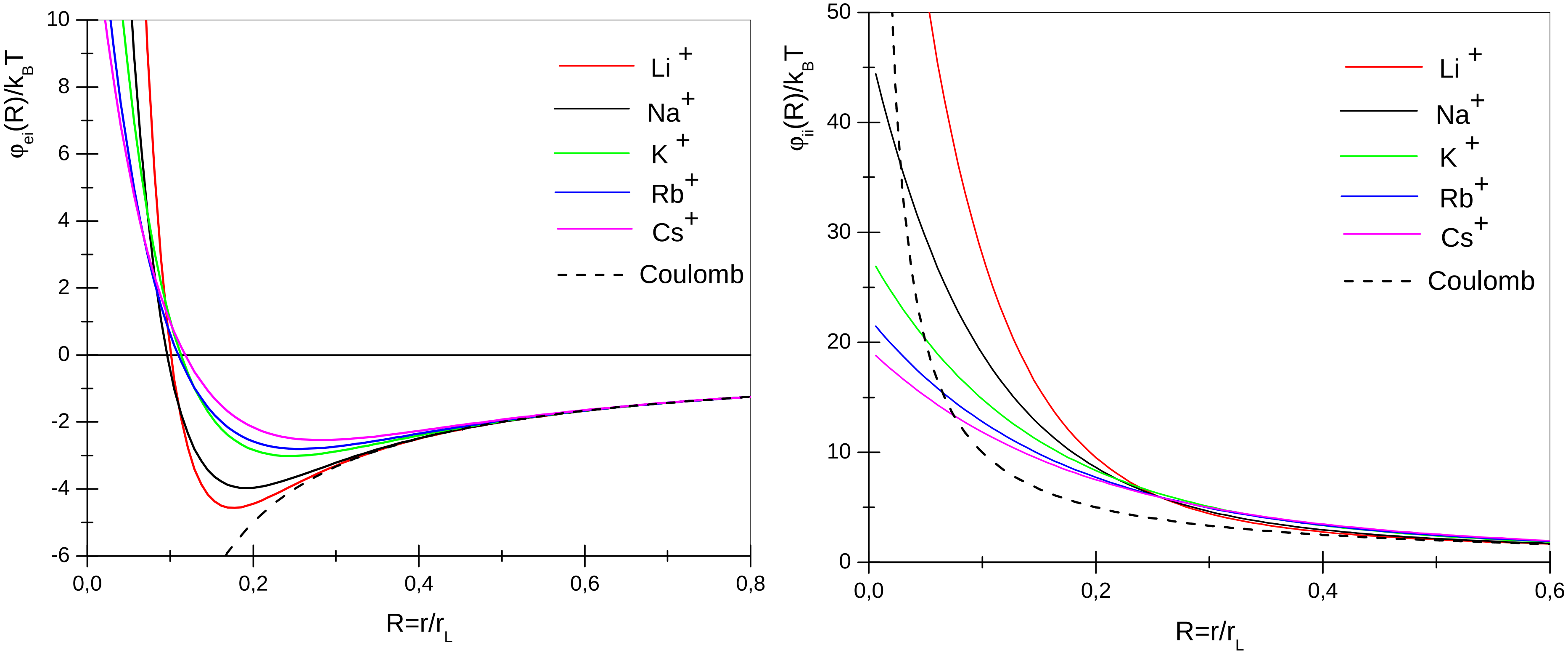




$$\varphi_{ii} = \frac{z^2e^2}{4\pi\varepsilon_0}\frac{1-e^{-r/R_{Cii}}}{r} + \frac{z^2e^2}{4\pi\varepsilon_0}\frac{a}{R_{Cii}}e^{-r/R_{Cii}}$$

z - Valency; a, $R_{Cii}=2R_{Cei}$ are adjustable to the optical spectra parameter

Hellmann-Gurskii-Krasko potential for alkali elements[3]



[3] Z. Gurski, G. Krasko, Proceedings of the USSR Academy of Sciences, 1971.V.197, Nr 4 (in russ.)

Screened Hellmann-Gurskii-Krasko Potential

Following [4] we solve: $\Delta_i \Phi_{ab}(\vec{r}_i^{\,a},\vec{r}_j^{\,b}) = \Delta_i \varphi_{ab}(\vec{r}_i^{\,a},\vec{r}_j^{\,b}) - \sum_{c=e,i}\frac{n_c}{k_B T}\int d\vec{r}_m^{\,c}\,\Delta_i \varphi_{ac}(\vec{r}_i^{\,a},\vec{r}_j^{\,c})\,\Phi_{cb}(\vec{r}_m^{\,c},\vec{r}_j^{\,b})$

where $\varphi_{ee}(r) = \frac{e^2}{4\pi\varepsilon_0}\frac{1-e^{-r/\lambda_{ee}}}{r} + k_B T \ln 2 e^{-r^2/(\lambda_{ee}^2 \ln 2)}$ - Deutsch potential

$\varphi_{ei}, \varphi_{ii}$ – Hellmann-Gurskii-Krasko potential

We derive the following expressions with the **constraint:** $\Gamma \lesssim 1$

$$\Phi_{ei}(k) = \frac{ze^2}{\varepsilon_0 \Delta}\frac{(2a-1)R_{Cei}^2 k^2 - 1}{k^2(1+k^2 R_{Cei}^2)^2},$$

$$\Phi_{ee}(k) = \frac{e^2}{\varepsilon_0 \Delta}\left\{\frac{1}{k^2(1+k^2\lambda_{ee}^2)} + \frac{1}{k^4 r_{Di}^2}\left[\frac{(2a+1)R_{Cii}^2 k^2 + 1}{(1+k^2\lambda_{ee}^2)(1+k^2 R_{Cii}^2)^2} - \left(\frac{(2a-1)R_{Cei}^2 k^2 - 1}{(1+k^2 R_{Cei}^2)^2}\right)^2\right] + A\left(1+\frac{(2a+1)R_{Cii}^2 k^2 + 1}{k^2 r_{Di}^2 (1+k^2 R_{Cii}^2)^2}\right)\exp\left(-\frac{k^2}{4b^2}\right)\right\},$$

$$\Phi_{ii}(k) = \frac{z^2 e^2}{\varepsilon_0 \Delta}\left\{\frac{(2a+1)R_{Cii}^2 k^2 + 1}{k^2(1+k^2 R_{Cii}^2)^2} + \frac{1}{k^4 r_{De}^2}\left[\frac{(2a+1)R_{Cii}^2 k^2 + 1}{(1+k^2\lambda_{ee}^2)(1+k^2 R_{Cii}^2)^2} - \left(\frac{(2a-1)R_{Cei}^2 k^2 - 1}{(1+k^2 R_{Cei}^2)^2}\right)^2\right] + A\frac{(2a+1)R_{Cii}^2 k^2 + 1}{k^2 r_{De}^2 (1+k^2 R_{Cii}^2)^2}\exp\left(-\frac{k^2}{4b^2}\right)\right\},$$

$$\Delta = 1 + \frac{1}{k^2 r_{De}^2 (1+k^2\lambda_{ee}^2)} + \frac{(2a+1)R_{Cii}^2 k^2 + 1}{k^2 r_{Di}^2 (1+k^2 R_{Cii}^2)^2} + \frac{1}{k^4 r_{De}^2 r_{Di}^2}\left[\frac{(2a+1)R_{Cii}^2 k^2 + 1}{(1+k^2\lambda_{ee}^2)(1+k^2 R_{Cii}^2)^2} - \left(\frac{(2a-1)R_{Cei}^2 k^2 - 1}{(1+k^2 R_{Cei}^2)^2}\right)^2\right] + \frac{A}{r_{De}^2}\left(1+\frac{(2a+1)R_{Cii}^2 k^2 + 1}{k^2 r_{Di}^2 (1+k^2 R_{Cii}^2)^2}\right)\exp\left(-\frac{k^2}{4b^2}\right)$$

- screened HGK potential

$$1/r_{Di}^2 = z^2 e^2 n_i/(\varepsilon_0 k_B T),$$
$$1/r_{De}^2 = e^2 n_e/(\varepsilon_0 k_B T),$$
$$b = (\lambda_{ee}^2 \ln 2)^{-1},$$
$$A = k_B T \ln 2 \pi^{3/2} b^{-3/2} \varepsilon_0 / e^2$$

Screened Hellmann-Gurskii-Krasko Potential

if $\lambda_{ee}, R_{Cei}, R_{Cii} << r_{De}, r_{Di}$, then for $e-i$ and $i-i$ interactions:

Screened e-i HGK in the Debye approximation:

$$\Phi_{ib}(r) = \frac{zee_b}{4\pi\varepsilon_0}\frac{e^{-r/r_D} - e^{-r/R_{Cei}}}{r} + \frac{|zee_b|}{4\pi\varepsilon_0}\frac{a}{R_{Cib}}e^{-r/R_{Cib}}, \quad b = e, i,$$

and for $e-e$ interaction we have:

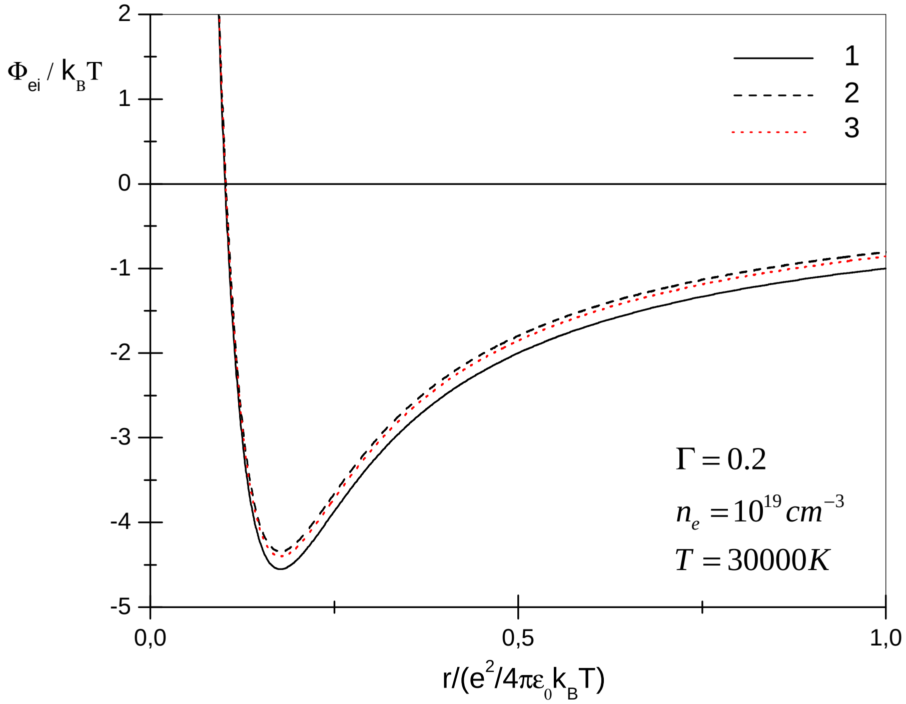
$$\Phi_{ee}(r) = \frac{e^2}{4\pi\varepsilon_0}\frac{e^{-r/r_D} - e^{-r/\lambda_{ee}}}{r} + k_B T \ln 2 e^{-r^2/(\lambda_{ee}^2 \ln 2)}$$

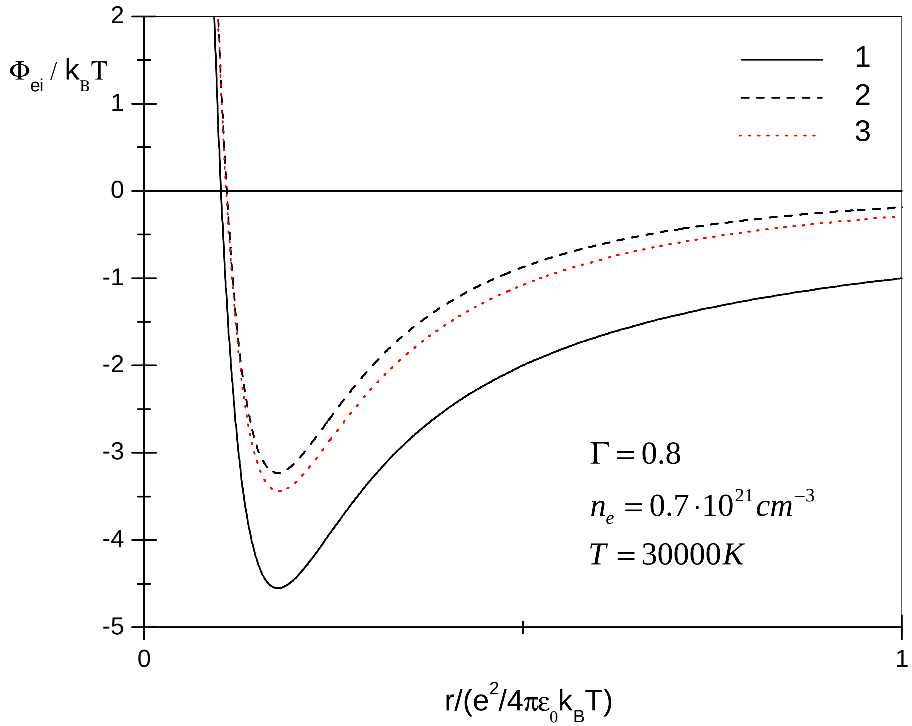
here $1/r_D^2 = \sum_{m=e,i} e_m^2 n_m /(\varepsilon_0 k_B T)$

[4] *Yu. V. Arkhipov, F.B. Baimbetov, A.E. Davletov, Eur.Phys. J. D* ***8****, 299-304 (2000)*

Screened Hellmann-Gurskii-Krasko Potential [5]

Electron-Ion Interaction





Comparison between the different e-i pseudopotentials of semiclassical Li^+-plasma : **1**: Hellmann-Gurskii-Krasko potential; **2**: Screened Hellmann-Gurskii-Krasko potential ; **3**: Screened HGK in a a Debye-Hückel approximation

[5] *S. P. Sadykova, W. Ebeling, I. Valuev and I. Sokolov, CPP.* ***49****, 76 – 89 (2009)*

A New Type of the Screened Hellmann-Gurskii-Krasko Potential

Following [4] we solve: $\Delta_i \Phi_{ab}(\vec{r}_i^{\,a},\vec{r}_j^{\,b}) = \Delta_i \varphi_{ab}(\vec{r}_i^{\,a},\vec{r}_j^{\,b}) - \sum_{c=e,i} \frac{n_c}{k_B T}\int d\vec{r}_m^{\,c}\, \Delta_i \varphi_{ac}(\vec{r}_i^{\,a},\vec{r}_j^{\,c})\Phi_{cb}(\vec{r}_m^{\,c},\vec{r}_j^{\,b})$

where $\varphi_{ee}(r) = \frac{e^2}{4\pi\varepsilon_0}\left\{\frac{1-e^{-r^2/\lambda_{ee}^2}}{r} + \frac{\sqrt{\pi}}{\lambda_{ee}}\left(1-erf\left(\frac{r}{\lambda_{ee}}\right)\right)\right\} - k_B T \tilde{A}_{ee}(\xi_{ee})\exp\left(-\frac{r^2}{\lambda_{ee}^2}\right)$ - Corrected Kelbg ! potential

$\varphi_{ei}, \varphi_{ii}$ – Hellmann-Gurskii-Krasko potential

We derive the following expressions with the **constraint:** $\Gamma \lesssim 1$

$$\Phi_{ei}(k) = \frac{ze^2}{\varepsilon_0 \Delta}\frac{(2a-1)R_{Cei}^2 k^2 - 1}{k^2(1+k^2R_{Cei}^2)^2},$$

$$\Phi_{ee}(k) = \frac{e^2}{\varepsilon_0 \Delta}\left\{\frac{2\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)}{k^3\lambda_{ee}}\int_0^{k\lambda_{ee}/2} e^{t^2}dt + \frac{1}{k^4 r_{Di}^2}\left[2\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\frac{(2a+1)R_{Cii}^2k^2+1}{k\lambda_{ee}(1+k^2R_{Cii}^2)^2}\int_0^{k\lambda_{ee}/2} e^{t^2}dt - \left(\frac{(2a-1)R_{Cei}^2k^2-1}{(1+k^2R_{Cei}^2)^2}\right)^2\right] + A\tilde{A}_{ee}(\xi_{ee})\left(1+\frac{(2a+1)R_{Cii}^2k^2+1}{k^2r_{Di}^2(1+k^2R_{Cii}^2)^2}\right)\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\right\},$$

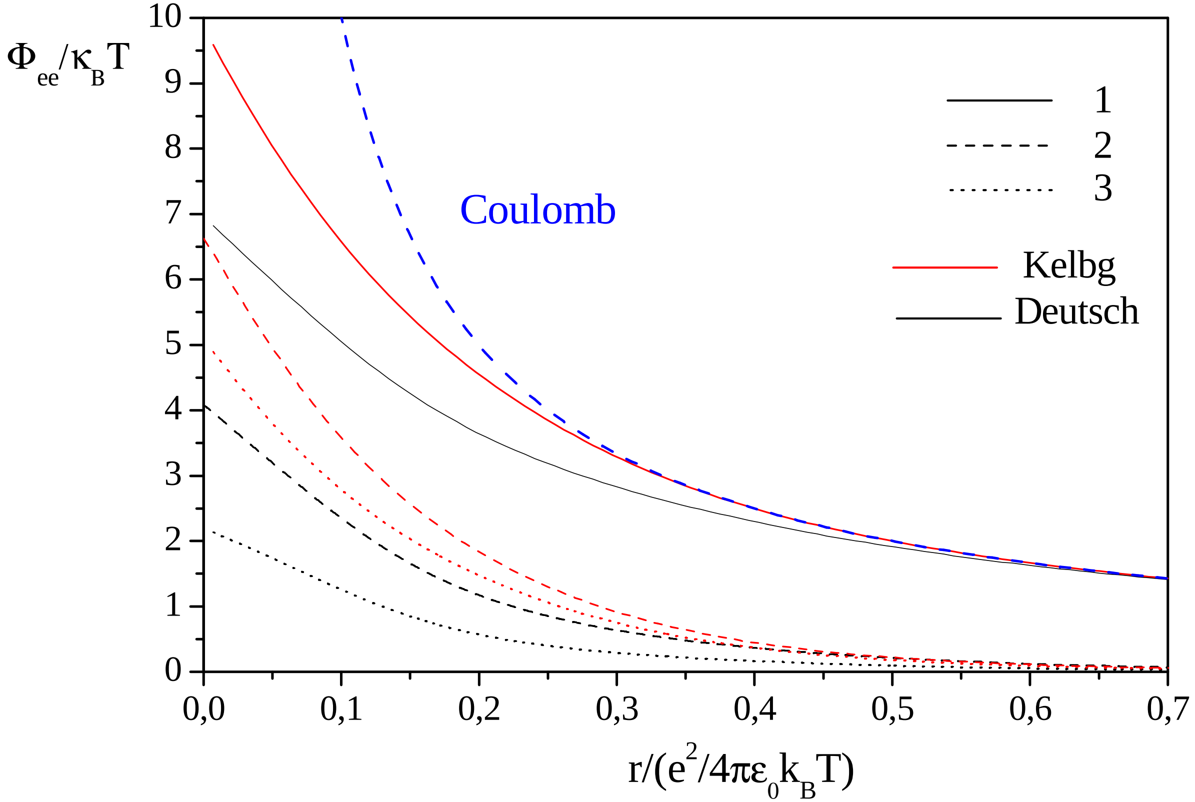
$$\Phi_{ii}(k) = \frac{z^2e^2}{\varepsilon_0 \Delta}\left\{\frac{(2a+1)R_{Cii}^2k^2+1}{k^2(1+k^2R_{Cii}^2)^2} + \frac{1}{k^4 r_{De}^2}\left[2\exp\left(-\frac{k^2\lambda_{ee}^2}{4}\right)\frac{(2a+1)R_{Cii}^2k^2+1}{k\lambda_{ee}(1+k^2R_{Cii}^2)^2}\int_0^{k\lambda_{ee}/2} e^{t^2}dt - \left(\frac{(2a-1)R_{Cei}^2k^2-1}{(1+k^2R_{Cei}^2)^2}\right)^2\right]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

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

- screened HGK potential

$$1/r_{Di}^2 = z^2e^2n_i/(\varepsilon_0 k_B T),$$
$$1/r_{De}^2 = e^2n_e/(\varepsilon_0 k_B T),$$
$$A = k_B T \pi^{3/2}\lambda_{ee}^3\varepsilon_0/e^2$$

Comparison of the new Hellmann-Gurskii-Krasko Potential with the Old One



Comparison between the different e-e pseudopotentials of semiclassical Cs^+-plasma at $T=8000$ K, $n_e=10^{26}$ **m^{-3}** : **1**: Hellmann-Gurskii-Krasko potential; **2**: **Screened** Hellmann-Gurskii-Krasko potential ; **3**: Screened HGK in a a Debye-Hückel approximation

EMD at location of an ion

According to Ortner's [6] theory for TCP plasma:

Fourier transform of EMD:

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

where $\phi(\vec{r}) = -il \cdot \vec{\nabla} V$, **here** $V(r) = e / 4\pi\varepsilon_0 r$

In the Debye Approximation:

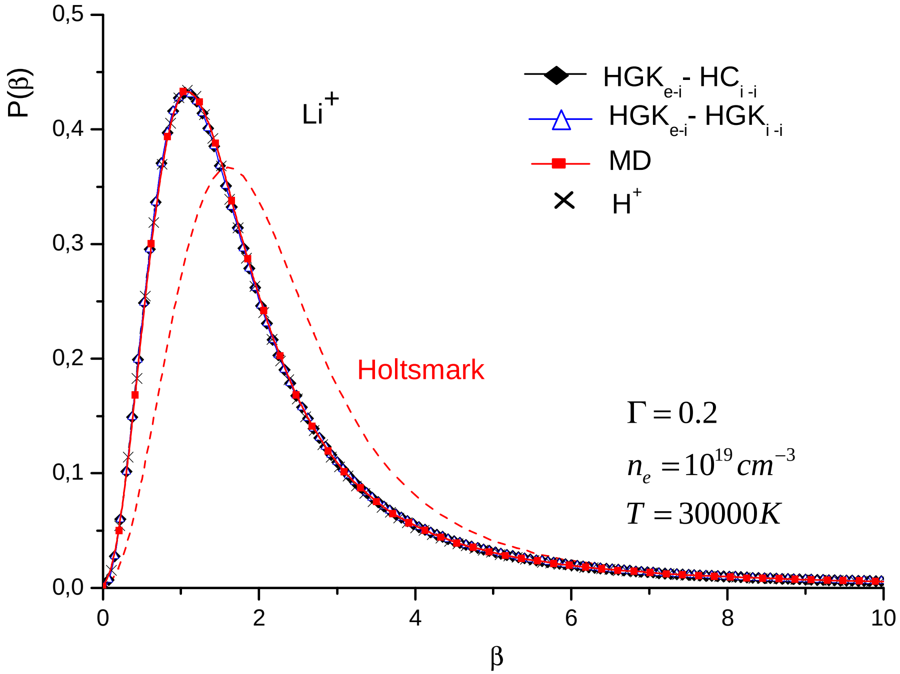
$$g_{ia}(\vec{r};\lambda) \cong g_{ia}(\vec{r},0) \exp\left\{ -i\lambda \hat{l} \cdot \vec{\nabla}_0 \frac{e_a}{4\pi\varepsilon_0 k_B T r} \exp(-\chi r) \right\},$$ **- Generalized RDF for the radiator**

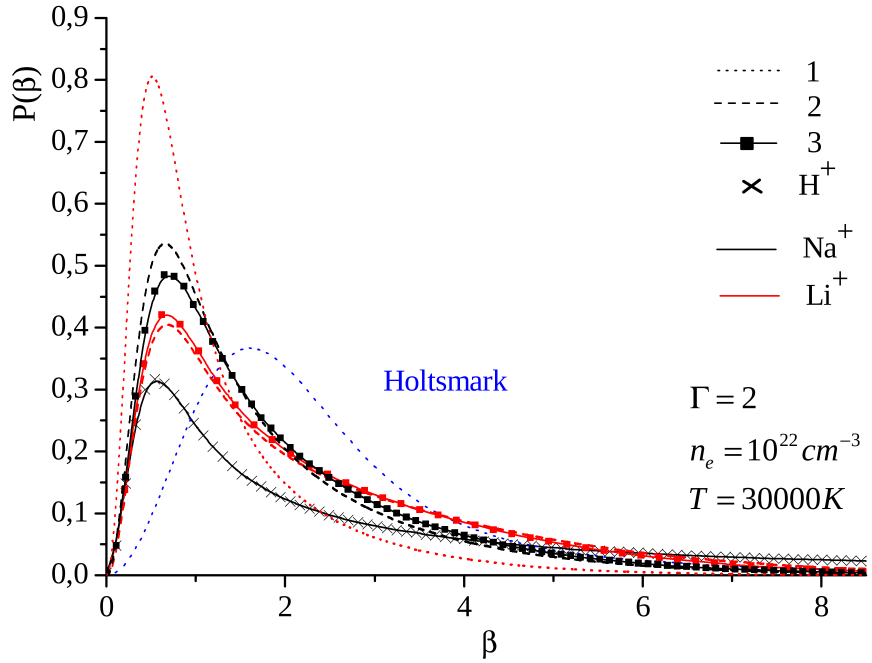
$$g_{ia}(r,0) = \exp\left\{ -\frac{\Phi_{ia}(r)}{k_B T} \right\}$$

$\Phi_{ia}(r)$ **-the screened HGK in the Debye or moderately coupled screened approximation**

[6] *J. Ortner, I. Valuev, W. Ebeling, Contrib. Plasma Phys.40, 555 (2000)*

EMD at Li^{+} - ion



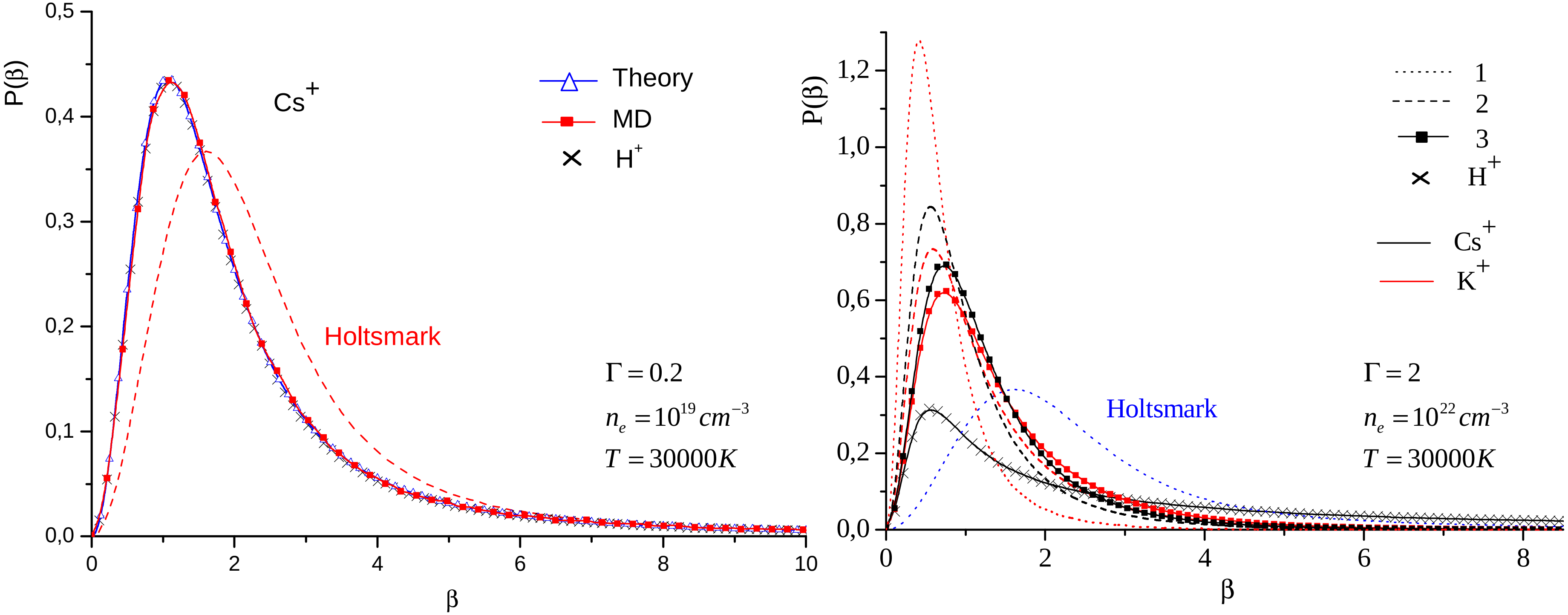


$$P(\beta) = \frac{2\beta}{\pi} \int_0^{\infty} l^* T(l^*) \sin(\beta l^*) dl^*,$$

where $\beta = \in / \in_0, l^* = l \in_0, \in_0 = e / 4\pi\varepsilon_0 r_0^{\,2}$

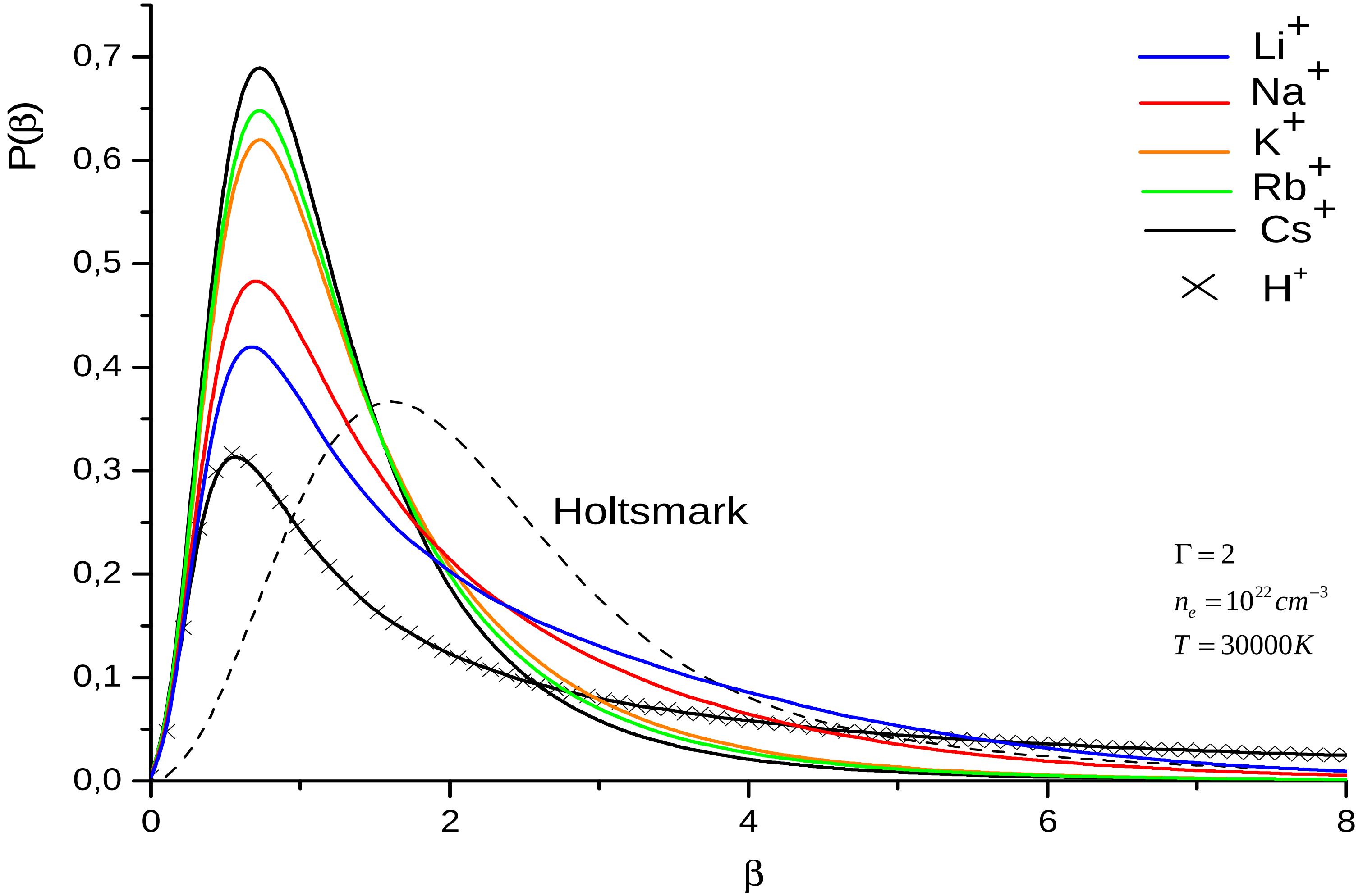
1: in the Debye approximation; **2**: in a moderately coupled screened HGK approximation; **3**: MC

EMD at Cs^+ - ion



1: in the Debye approximation; **2**: in a moderately coupled screened HGK approximation; **3**: MC

EMD in Alkali Plasmas at an ion [6]



6 S. P. Sadykova, W. Ebeling, I. Valuev and I. Sokolov, CPP 49, 388 (2009)

The Tails of EMD

At $\Gamma \to 0$ ⟶ **Holtsmark distribution:**

$$P(\beta) = \frac{2\beta}{\pi}\int_0^\infty l\exp(-l^\alpha)\sin(l\beta)dl \quad \text{with} \quad \alpha = 3/2$$

At $\beta \to \infty$ ⟶ $P(\beta) \propto 1.496\beta^{-\alpha-1} = 1.496\beta^{-5/2}$

At $\Gamma \to \infty$ ⟶ **Mayer distribution:**

$$P(\beta) = \sqrt{2/\pi}\,\Gamma^{3/2}\beta^2\exp(-\Gamma\beta^2/2)$$

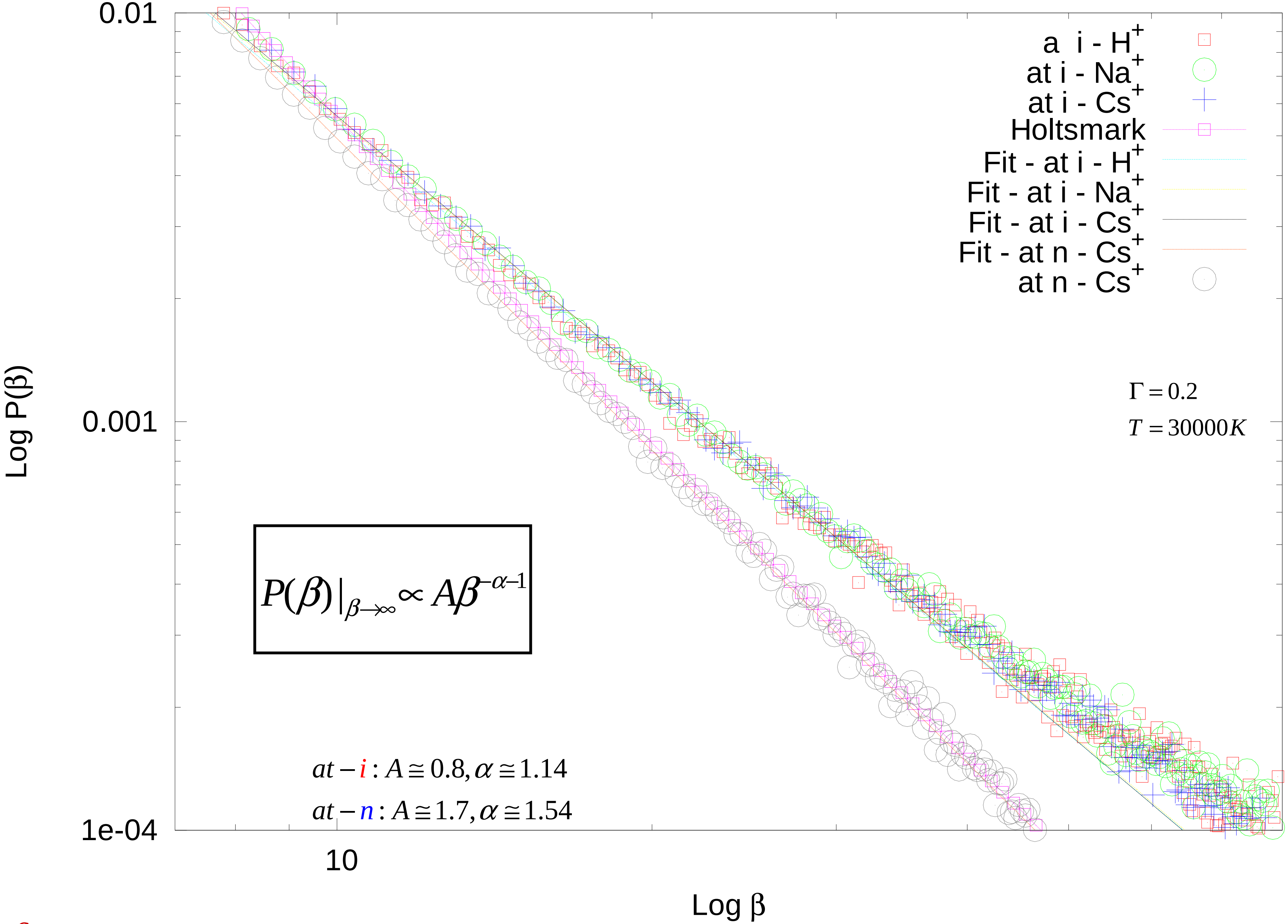
Fails in the strong-field limit !

A. Y. Potekhin's* asymptote:

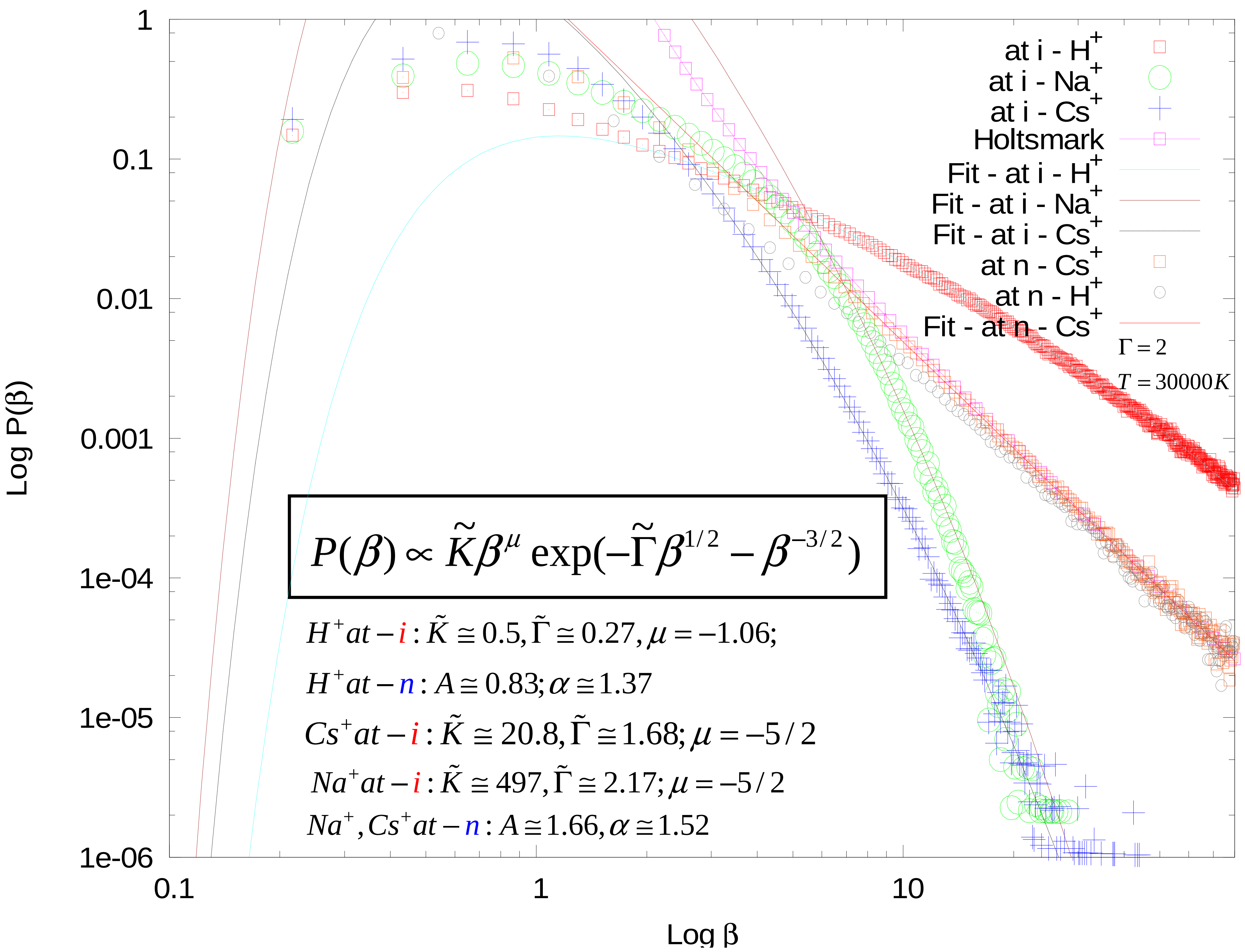
$$P(\beta) \propto \tilde{K}\beta^{-5/2}\exp(-\tilde{\Gamma}\beta^{1/2} - \beta^{-3/2})$$

is more accurate !

* *A. Y. Potekhin et al., Phys. Rev.E, V. 65, 036412*



[6] *S. P. Sadykova, W. Ebeling, I. Valuev and I. Sokolov, CPP 49, 388 (2009)*



Log P(β)
Log β
1
0.1
0.01
0.001
1e-04
1e-05
1e-06
0.1
1
10
at i - H+
at i - Na+
at i - Cs+
Holtsmark
Fit - at i - H+
Fit - at i - Na+
Fit - at i - Cs+
at n - Cs+
at n - H+
Fit - at n - Cs+
Γ = 2
T = 30000K
P(β) ∝ K̃β^μ exp(−Γ̃β^{1/2} − β^{−3/2})
H+ at − i : K̃ ≅ 0.5, Γ̃ ≅ 0.27, μ = −1.06;
H+ at − n : A ≅ 0.83; α ≅ 1.37
Cs+ at − i : K̃ ≅ 20.8, Γ̃ ≅ 1.68; μ = −5/2
Na+ at − i : K̃ ≅ 497, Γ̃ ≅ 2.17; μ = −5/2
Na+, Cs+ at − n : A ≅ 1.66, α ≅ 1.52

The Static Structure Factors. X-ray Thomson Scattering [7]

$$S_{ab}(k) = \delta_{ab} - \sqrt{\frac{n_a n_b}{k_B T_{ab}'}} \Phi_{ab}(k) - \delta_{ea}\delta_{eb}\left(\frac{T_e'}{T_i'} - 1\right)\frac{|q(k)|^2}{z} S_{ii}(k), \quad [8]$$

where

$$q(k) = \sqrt{z}\,\frac{S_{ei}(k)}{S_{ii}(k)}, \quad T_{ab}' = \frac{m_b T_a' + m_a T_b'}{m_a + m_b}$$

$$T_e' = \sqrt{T_e^2 + T_q^2}, \quad T_q = \frac{T_F}{1.3251\text{-}0.1779\sqrt{\mathrm{r_s}}}$$

$$T_i' = \sqrt{T_i^2 + \frac{3}{2}\pi^2 T_D^2}, \quad T_D = \frac{\hbar\Omega_{pi}}{k_B},$$

$$\Omega_{pi} = \frac{\omega_{pi}}{\sqrt{1 + k_F^2 / k_0^2}} \qquad k_0 = (2/Z_f)^{1/3} k_F$$

$\Phi_{ab}(k)$ **- screened HGK potential**

$$S_{ZZ}(k,\omega) = -\frac{\hbar\,\mathrm{Re}\,\varepsilon^{-1}(k,\omega)}{\pi\Phi(k)[1 - \exp(-\beta\hbar\omega)]}, \quad [9]$$

$$\Phi(k) = \frac{4\pi e^2}{4\pi\varepsilon_0 k^2}$$

$\varepsilon^{-1}(k,\omega)$ **- The Nevanlinna formula of the theory of moments**

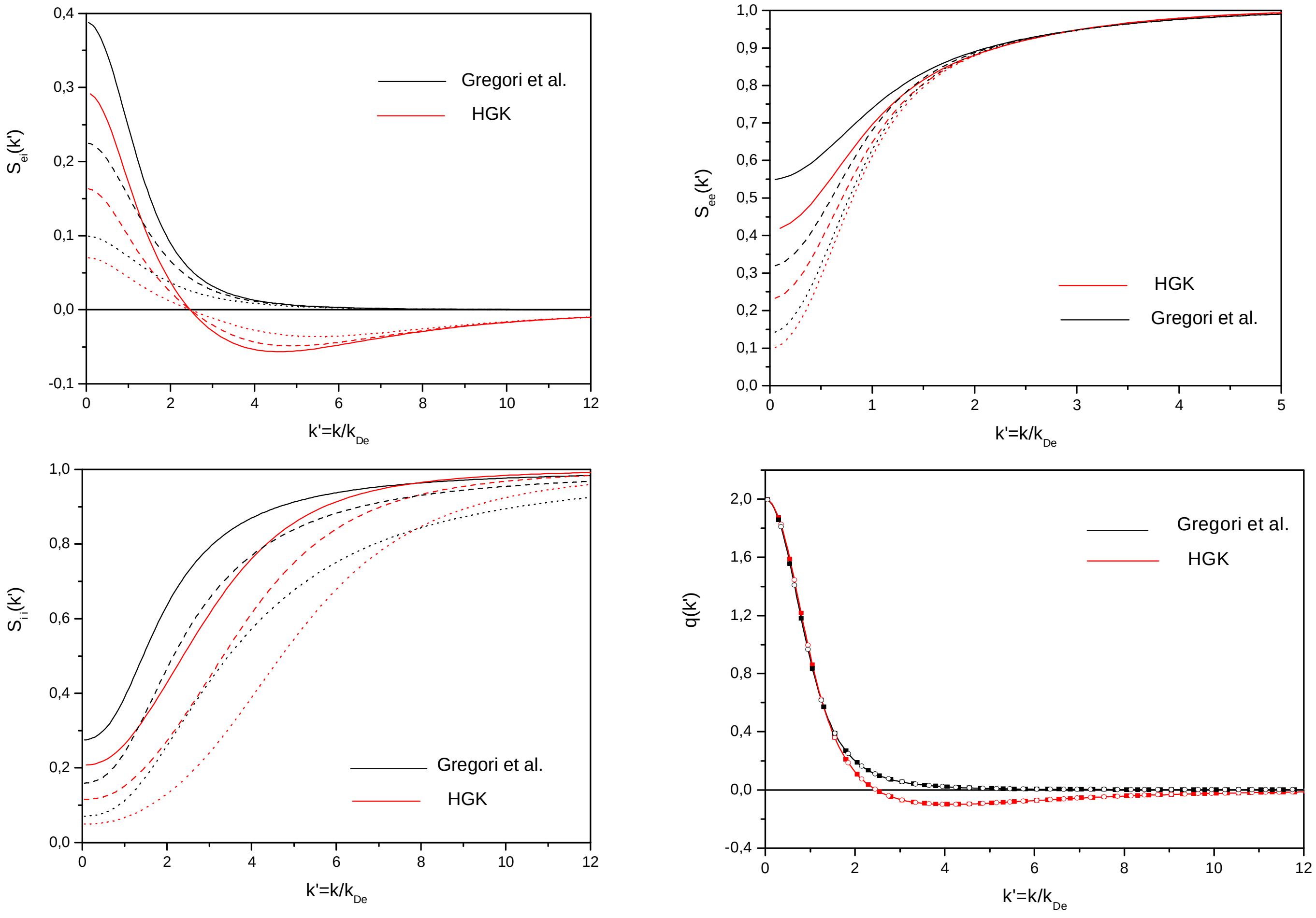
$\varepsilon^{-1}(k,\omega)$ **- is determined through the HGK potential**

[7] *Gregori, Glenzer S. H., O. S. Landen, Phys. Rev. E 74, 026402 (2006)*

[8] *P. Seuferling, J. Vogel, C. Toepffer, Phys. Rev. A. 40, 323 (1989)*

[9] *V. M. Adamyan, I. M. Tkachenko, High. Temp. (USA) 21, 307 (1983); Sov. J. Plasma Phys. 11, 481 (1985)*

The Static Structure Factors for Be^{2+}- plasma



T_e=20 eV,
n_e=2.5 10^{23} m^{-3}

Solid line: T_i/T_e=1; ***Dashed line***: Ti/Te=1; ***Dotted line***: Ti/Te=0.2

Summary

- The EMD at the location of an ion and neutral point have been calculated using coupling parameter integration technique for Alkali plasmas proposed by Ortner et al. and compared with MD and MC simulations. The EMD are studied in a frame of the Hellmann-Gurskii-Krasko pseudopotential model which takes into account the ion structure. For determination of RDF the screened HGK potential in the Debye and moderately coupled screened approximation have been used, where the latter shows good agreement with MC at moderately large Γ.

- With increasing of Γ the ion core structure starts to play significant role and influences the EMD very much

- The tails of the EMDs at an ion at low Γ or neutral point are in all cases of Levy type, but with the different exponents depending on the density and temperature of plasma. The long tails at a neutral point are compatible with the Holtsmark‘s tail.

- At high values of Γ the EMD tails measured at an ion obey to the Potekhin law.

- The high-field tails for Alkali-plasmas decay much faster than the fields acting on protons in hydrogen plasmas.

- The screened HGK model can be used for determination of the static and dynamic structure factors for X-ray Thomson scattering applications