The electrostatic interaction of two point charges in equilibrium plasmas within the Debye approximation

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Abstract. This paper is devoted to a careful study of two charge interaction in an equilibrium plasma within the Debye approximation. The effect of external boundary conditions for the electric field strength and potential on the electrostatic force is studied. The problem is solved by the method of potential decomposition into Legendre polynomials up to the fifth multipole term included. It is shown that the effect of attraction of identically charged macroparticles is explained by the influence of the external boundary. When the size of a calculation cell is increased the attraction effect disappears and the electrostatic force is well described by the screened Debye–Hückel potential.

1. Introduction

In paper [1], the electrostatic force between two charged macroparticles in a plasma was considered using the Maxwell stress tensor. It was shown that within the Poisson-Boltzmann model two macroparticles with the same charge always repulsed each other in both isothermal and nonisothermal plasmas. Ignatov in [2] deduced the same result (see also [3–5]). In spite of this clear conclusion new papers are regularly published with the statement of the attraction of macroparticles with charges of the same sign in the equilibrium plasma (see, for example, papers [6–8]). This paper is devoted to a careful study of the electrostatic interaction of two charged macroparticles in the equilibrium plasma within the Poisson-Boltzmann model using the Debye-Hückel approximation.

2. Interaction force of two charges within the Poisson-Boltzmann model

In the Poisson-Boltzmann model, the electron and ion density distributions are described by the Boltzmann law

$$n_e = n_{e,0} \exp\left(\frac{e\phi}{T_e}\right), \quad n_i = n_{i,0} \exp\left(-\frac{e\phi}{T_i}\right), \tag{1}$$

and $n_{e,0} = n_{i,0} \equiv n_0$ as follows from the quasi-neutrality condition and finiteness of charges q. For the isothermal case $T_e = T_i \equiv T$, in paper [1] using the Maxwell stress tensor it was obtained

$$F_z = -\int\limits_0^\infty \left\{ \tfrac{1}{4} E_s^2 + 4\pi n_0 T \left[\cosh\left(\frac{e\phi_s}{T}\right) - 1 \right] \right\} r_z dr_z, \tag{2}$$

here F_z is the interaction force of two point charges in the equilibrium plasma, z and r_z are the coordinates in the cylindrical frame system with the origin in the center of the first particle and z-axis directed to the center of the second one, E_s and ϕ_s are the electric field strength and potential in the plane $z = \frac{1}{2}R_{\text{int}}$, R_{int} is the interparticle distance.

The minimum of the hyperbolic cosine is equal to 1. Therefore, the expression in the square brackets and, correspondingly, the expression in braces in Eq. (2) are always positive (or equal to zero only when the potential and field strength in the symmetry plane of the problem are zero, which is possible only for the case of zero charges; however, this case is of no interest). For this reason, $F_z < 0$ at any distances between the particles; i.e., the same sign charged dust particles in a plasma with the Boltzmann distributions of the electron and ion number densities always repulse each other. It is worth noting that a similar expression (taking into account the neutralizing background being equal to zero) for this force was derived by a different method in [2]. We also note that the absence of attraction between two charged plates in the equilibrium plasma in one-dimensional plane geometry was proved by Derjaguin [9].

For a nonisothermal plasma, expanding exponentials into the Taylor series Filippov et al. [1] obtained

$$F_z = -\frac{1}{4}\int\limits_0^\infty \left\{ E_s^2 + 4\pi n_0 \left(e\phi_s\right)^2 \left(\frac{1}{T_i} + \frac{1}{T_e}\right) - \frac{8\pi}{3!} n_0 \left(e\phi_s\right)^3 \left(\frac{1}{T_i^2} - \frac{1}{T_e^2}\right) + ... \right\} r_z dr_z. \tag{3}$$

It is seen that, for $T_e \geq T_i$ and the negative potential ϕ_s (i.e., for negatively charged macroparticles), the terms of odd ϕ_s powers, as well as the terms of even powers, are positive. For this reason, identically charged dust particles in nonisothermal plasma also repulse each other.

The final analytical expression for the force can be derived under the condition $|\phi_s/T| \ll 1$. In this case, it follows from Eqs. (2) and (3) that

$$F_z = -\frac{1}{4}\int\limits_0^\infty \left(E_s^2 + k_D^2 \phi_s^2\right) r_z dr_z, \tag{4}$$

where k_D is the inverse Debye radius: $k_D^2 = 4\pi e^2 n_0 \left(T_i^{-1} + T_e^{-1}\right)$. Further, we assume that the macroparticles are point-like. Integrating Eq. (4) with Debye potential, it was derived in [1]

$$F_z = -\frac{e^2 q^2}{R_{\text{int}}^2}\left(1 + k_D R_{\text{int}}\right) e^{-k_D R_{\text{int}}}. \tag{5}$$

Substituting this expression into the relation $F_z = -\nabla U$ and integrating the latter by taking into account that the interaction energy at $R_{\text{int}} = \infty$ vanishes, authors [1] arrived at the expression

$$U = \frac{e^2 q^2}{R_{\text{int}}} e^{-k_D R_{\text{int}}} \tag{6}$$

for the electrostatic interaction energy of two macroparticles. According to Eqs. (5) and (6), the force and interaction potential of two macroparticles are described by the Yukawa potential and the identically charged macroparticles repulse each other.

3. Helmholtz free energy of the two macroparticles in the canonical ensemble

The authors of [15–18] draw a wrong conclusion on the electrostatic attraction between two macroparticles with charges of the same sign, because they use the internal energy to determine the force. It is known [10] that the internal energy is the thermodynamic potential in terms of the entropy S and volume V, whereas the Helmholtz free energy is the thermodynamic potential in terms of the temperature T and volume V in the canonical ensemble. For this reason, the Helmholtz free energy should be used to determine the force for isothermal processes [10]. The Helmholtz free energy of the system of two macroparticles in an infinite plasma was defined in [1] using the internal energy part depending on the distance between macroparticles obtained in [15–20] in the form

$$\mathcal{E}\left(R_{\rm int}\right) = \frac{e^2 q_1 q_2}{R_{\rm int}}\left(1 - \tfrac{1}{2}k_D R_{\rm int}\right) e^{-k_D R_{\rm int}}, \tag{7}$$

where q_1, q_2 are the charges of the macroparticles. Only the screening constant $k_D = \mathrm{const}{\cdot}T^{-1/2}$ is a function of temperature in Eq. (7). Using the thermodynamic identity [10]

$$\mathcal{F} = T\int\limits_T^{\infty}\left(\frac{\mathcal{E}}{T^2}\right)_V dT, \tag{8}$$

from Eq. (7) the authors of [1] derived

$$\mathcal{F} = \frac{e^2 q_1 q_2}{R_{\rm int}}\, e^{-k_d R_{\rm int}}. \tag{9}$$

For the case of identical charges, this expression coincides with Eq. (6); hence, the interaction between two macroparticles in the equilibrium plasma is potential. Moreover, the final conclusion is that the electrostatic attraction between two identically charged particles is absent in the Poisson-Boltzmann model under any conditions.

4. Entropy of the system of two charged macroparticles in equilibrium plasma

To finally clarify the question let us calculate the electron and ion entropy in the considered system that is determined for the ideal gas of electrons and ions by the following expression [10]:

$$S = S_e + S_i = -\sum_{\sigma=e,i}\int n_\sigma(\mathbf{r},\mathbf{p})\left[\ln n_\sigma\left(\mathbf{r},\mathbf{p}\right) - 1\right]\frac{d\mathbf{r}d\mathbf{p}}{\left(2\pi\hbar\right)^3}, \tag{10}$$

where $n_\sigma(\mathbf{r},\mathbf{p})$ are the electron and ion distribution functions which are expressed in the equilibrium plasma as

$$n_\sigma(\mathbf{r},\mathbf{p}) = e^{(\mu_\sigma - \varepsilon_\sigma)/T}, \tag{11}$$

μ_σ is the chemical potential, ε_σ is the total energy:

$$\varepsilon_\sigma = \frac{\mathbf{p}^2}{2m_\sigma} + e_\sigma\phi(\mathbf{r}).$$

The chemical potential can be found from the normalization condition

$$N_\sigma = \int n_\sigma(\mathbf{r},\mathbf{p})\frac{d\mathbf{r}d\mathbf{p}}{\left(2\pi\hbar\right)^3}, \tag{12}$$

where N_σ is the total number of particles of the plasma σ-component. So we have

$$\mu_\sigma = T\ln\left(\frac{\vartheta_{0\sigma}N_\sigma}{\int e^{-e_\sigma\phi/T}d\mathbf{r}}\right), \tag{13}$$

where $\vartheta_{0\sigma} = (2\pi\hbar^2/m_\sigma T)^{3/2}$. For non-disturbed plasma ($\phi = 0$) we have:

$$S_{0\sigma} = -N\left[\ln\left(\vartheta_{0\sigma} n_0\right) - \tfrac{5}{2}\right]. \tag{14}$$

For the entropy addition connected with the electrostatic interaction, we now obtain:

$$\Delta S_\sigma = S - S_{0\sigma} = N_\sigma\left[\ln\left(\frac{1}{V}\int e^{-e_\sigma\phi/T}d\mathbf{r}\right) + \frac{\int\frac{e_\sigma\phi}{T}\,e^{-e_\sigma\phi/T}d\mathbf{r}}{\int e^{-e_\sigma\phi/T}d\mathbf{r}}\right]. \tag{15}$$

where V is the system volume. It is well known that when the condition $|e\phi_{1,2}/T| \ll 1$ is fulfilled the screened potential is described by the Debye-Hückel solution [11]

$$\phi_i = \frac{eq_i}{|\mathbf{r}-\mathbf{r}_i|}e^{-k_D|\mathbf{r}-\mathbf{r}_i|}, \tag{16}$$

where $\mathbf{r}_i$ is the position of the i-th charged macroparticle, ϕ_1 and ϕ_2 are the potential distributions of the bulk charges connected with the first and second macroparticles (including their charges), respectively. Let us pay particular attention to the fact that the solution (16) was found within the linear approximation of ratios $e\phi_{1,2}/T$, therefore, in the decomposition of $e^{-e_\sigma\phi/T} = e^{-e_\sigma\phi_1/T}e^{-e_\sigma\phi_2/T}$ in (15) we should only keep the linear term.

In this case we get from (15):

$$\begin{aligned}\Delta S_\sigma &= \frac{N_\sigma}{V}\int\left(-\frac{e_\sigma\phi_1}{T} - \frac{e_\sigma\phi_2}{T} + \frac{e^2\phi_1\phi_2}{T^2}\right)d\mathbf{r} + \frac{N_\sigma}{V}\left(\frac{e_\sigma}{T}\int\phi d\mathbf{r} - \frac{e^2}{T^2}\int\phi^2 d\mathbf{r}\right)\\ &\equiv \frac{e^2N_\sigma}{VT^2}\int\left(\phi_1\phi_2 - \phi^2\right)d\mathbf{r}.\end{aligned} \tag{17}$$

From (17) the depending on the interparticle distance part of the entropy addition is as follows:

$$\Delta S_\sigma\left(R_{\text{int}}\right) = -\frac{e^2n_0}{T^2}\int\phi_1\phi_2 d\mathbf{r} = -\tfrac{1}{4}\frac{k_D}{T}e^{-k_DR_{\text{int}}}. \tag{18}$$

Finally, for the addition to the entropy we obtain

$$\Delta S\left(R_{\text{int}}\right) = \Delta S_e\left(R_{\text{int}}\right) + \Delta S_i\left(R_{\text{int}}\right) = -\tfrac{1}{2}\frac{k_D}{T}e^{-k_DR_{\text{int}}}. \tag{19}$$

Now after the substitution of Eqs. (7) and (19) into the thermodynamical equality [10]

$$\mathcal{F} = \mathcal{E} - TS, \tag{20}$$

we get the following expression

$$U = \frac{e^2q_1q_2}{R_{\text{int}}}e^{-k_DR_{\text{int}}} \tag{21}$$

that exactly coincides with Eq. (6) in the case of two equal charges. This shows that the minimum in the dependence of the electrostatic energy for the system of two charged macroparticles in plasma on the distance between them is formed owing to the change in the system entropy, that is, due to the energy exchange with the thermostat.

5. Influence of the external boundary upon interaction of two macroparticles

In papers [21,22] the energy of the electric field of two charged macroparticles in non-equlibrium plasma was calculated and the minimum in the dependence of this energy on the interparticle distance was found. On the basis of this observation a mistaken conclusion was made about the attraction of similarly charged macroparticles. In paper [20] the electric field energy and using the Maxwell tension tensor the electrostatic interaction force was calculated for two similarly charged macroparticles in the non-equilibrium plasma created by an external gas ionization source. It was shown that the energy of the electric field had the minimum as a function of the interparticle distance, there being no attraction force between similarly charged macroparticles, in full compliance with the previous section.

In paper [8] the effect of attraction of similarly charged macroparticles was also revealed, but in that case the range of distances where the effect was observed was much less than the Debye radius. In that range the interaction of two particles is close to the Coulomb one and no attraction effect should be observed if the surface charge polarization (for example, see [23–26]) which was not taken into account in [8] is not considered. In our opinion the attraction effect in [8] appeared owing to the wrong choice of the arbitrary constant of the potential and to the use of the quasineutrality condition in the approximate form.

In [8] the authors state that in [1, 3] the absence of attraction was only proved for non-quasineutral systems. The incorrectness of this statement can easily be seen by integrating the bulk charge in the spherical coordinate system with the pole in the center of the considered particle. For a bulk charge connected with the i-th particle we get using (16):

$$Q_i = -\int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} \frac{k_D^2}{4\pi e}\phi_i r_i^2 dr d\theta_i d\varphi_i = -\int_0^{\infty} \frac{q_i}{r_i} e^{-k_D r_i} k_D^2 r_i^2 dr_i = -q_i \int_0^{\infty} e^{-\tilde{r}_i} \tilde{r}_i d\tilde{r}_i = -q_i, \tag{22}$$

that is, each charge system is quasineutral.

In paper [7] the interaction of two macroparticles was considered with approximate account of polarization effects of the surface charge, the attraction appearing at distances compared with the Debye screening radius R_D . Unfortunately, the size of particle was not given in paper [7], and the variable that at first denoted the radius of macroparticles meant the dimensionless distance in the section where the results were discussed. If the size of macroparticles was less than the Debye radius the polarization effects could not lead to the attraction effects at distances about R_D (see [23–26]). Baimbetov et al. in [7] state that in [1] the dependence of the static longitudinal dielectric function $\epsilon_L(k, 0)$ on the wavevector k was neglected. In reality in [1] the interaction was considered without using the plasma dielectric function. If the interaction of two macroparticles is considered with using the $\epsilon_L(k, 0)$ in the Debye approximation [27]

$$\epsilon_L(k, 0) = 1 + \frac{k_D^2}{k^2}, \tag{23}$$

one obtains for the Fourier transform of the interaction potential

$$U(k) = \frac{4\pi e^2 q_1 q_2}{k^2} \frac{1}{\epsilon_L(k, 0)} = \frac{4\pi e^2 q_1 q_2}{k^2 + k_D^2}. \tag{24}$$

Here $4\pi e^2 q_1 q_2/k^2$ is the Fourier transform of the Coulomb potential for macroparticles with the charges q_1 and q_2 in elementary charges. After the inverse transformation of Eq. (24) we obtain Eq. (21) for the interaction potential.

In papers [28, 29] the electrostatic interaction force of two macroparticles was calculated on the basis of numerical simulation with the use of the Maxwell tension tensor and the attraction of two similarly charged macroparticles was found. The calculation was performed for the finite cell with an external boundary. To reveal the influence of the external boundary let us consider the interaction of two charged macroparticles of a small radius $k_D a_1 \ll 1$, $k_D a_2 \ll 1$ in equilibrium plasma. Here a_1 and a_2 are the radius of the macroparticles, $k_D = \sqrt{4\pi e^2 \left(n_{e0} + n_{i0}\right)/T}$ is the Debye screening constant, T is the temperature of electrons and ions in energetic units, e is the absolute value of the electron charge, n_{e0} and n_{i0} are the concentrations of electrons and ions in the non-disturbed plasma.The geometry of the interaction in the spherical coordinate system is given in figure 1. The self-consistent potential of macroparticles and plasma will be determined on the basis of the linearized Poisson-Boltzmann equation [11]:

$$\triangle\phi - k_D^2\phi = 4\pi e\left(n_{e0} - n_{i0}\right), \tag{25}$$

Owing to the linearity of the considered problem, the total potential can be represented as a superposition of potentials for systems of charges connected with each macroparticle:

$$\phi\left(r,\theta\right) = \phi_1\left(r_1,\theta_1\right) + \phi_2\left(r_2,\theta_2\right). \tag{26}$$

Let us find the solution in the finite cell whose external boundary is the sphere with the center in the point O and with the radius R_b. Here we will not take into account the effects connected with the size of particles, therefore, the limit transition $a_1 \to 0$, $a_2 \to 0$ is implied everywhere below. Let us impose the following boundary conditions upon the system:

$$\left.\frac{\partial\phi_1\left(r_1,\theta_1\right)}{\partial r_1}\right|_{r_1=a_1} = -\frac{eq_1}{a_1^2}, \quad \left.\frac{\partial\phi_2\left(r_2,\theta_2\right)}{\partial r_2}\right|_{r_2=a_2} = -\frac{eq_2}{a_2^2}; \tag{27}$$

$$\left.\phi\left(r,\theta\right)\right|_{r=R_b} = 0, \quad \left.\frac{\partial\phi\left(r,\theta\right)}{\partial r}\right|_{r=R_b} = 0. \tag{28}$$

The boundary conditions (28) were used in [29].

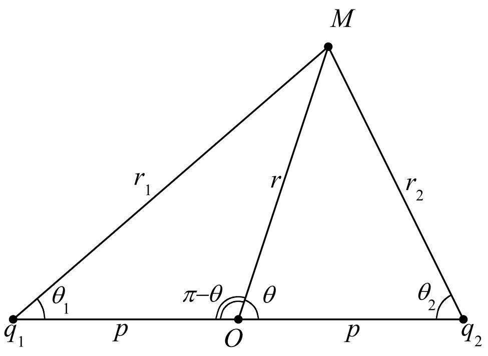

Figure 1. Geometry of the electrostatic interaction of two charged macroparticles. r_i, θ_i $(i = 1, 2)$ are the radius and polar angle in the spherical frame system with the pole in the center of i-th macroparticle and with the axe directed to the center of the other macroparticle, $R_{\rm int} = 2p$ is the interparticle distance, q_1, q_2 are the charges of the macroparticles.

Here we should discuss the conditions at the external boundary. The second condition (28) provides the quasineutrality in the considered cell, and the first condition results from the fact that in the Poisson-Boltzmann model the distribution of electrons and ions is according to the Boltzmann law:

$$n_e = n_{e0}e^{e\phi/T_e}, \quad n_i = n_{i0}e^{-e\phi/T_i}. \tag{29}$$

Therefore, the arbitrary constant of the potential had already been chosen: it was $\phi = 0$ where $n_e = n_{e0}$ and $n_i = n_{i0}$. In a case of the infinite calculation cell there are no problems with choosing the arbitrary constant of the potential, since in this case $n_{e0} = n_{i0}$. In case of the finite cell we have $n_{e0} \neq n_{i0}$ (for example, if the external boundary is rather close, then the condition $n_{e0} \ll n_{i0}$ will be satisfied) and after the linearization of the Boltzmann distribution in the Poisson equation there will be a constant term given in (1). The arbitrary constant of the potential should be determined by integrating the linearized distributions of electrons and ions and using the quasineutrality condition:

$$2\pi \int_0^{R_b} \int_{-1}^{1} \left[n_{e0} - n_{i0} + \frac{k_D^2}{4\pi e} \phi(r,\mu) \right] r^2 dr d\mu = q_1 + q_2. \tag{30}$$

In a case of the finite cell the general solution of Eq. (25) for the distribution of the potentials $\phi_1(r_1,\theta_1)$ and $\phi_2(r_2,\theta_2)$ with the axial symmetry taken into account is as follows [12]:

$$\phi_1(r_1,\theta_1) = \sum_{n=0}^{\infty} \left[A_n \frac{K_{n+1/2}(\tilde{r}_1)}{\sqrt{\tilde{r}_1}} + B_n \frac{I_{n+1/2}(\tilde{r}_1)}{\sqrt{\tilde{r}_1}} \right] P_n(\cos\theta_1) + G_1, \tag{31}$$

$$\phi_2(r_2,\theta_2) = \sum_{n=0}^{\infty} \left[C_n \frac{K_{n+1/2}(\tilde{r}_2)}{\sqrt{\tilde{r}_2}} + D_n \frac{I_{n+1/2}(\tilde{r}_2)}{\sqrt{\tilde{r}_2}} \right] P_n(\cos\theta_2) + G_2, \tag{32}$$

where $\tilde{r}_i = k_D r_i$, $i = 1,2$; $I_{n+1/2}$, $K_{n+1/2}$ are the modified Bessel functions of the first kind and of the third kind respectively; P_n are the Legendre polynomials, r_1, r_2 are the lengths of the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, A_n, B_n, C_n, D_n, $n = 0,1,\ldots,\infty$ are the coefficients which are determined by the boundary conditions (27,28), and the coefficients G_1 and G_2 are necessary to compensate the constant term in Eq. (25).

For small argument the modified Bessel functions are determined by the expressions [13]:

$$K_{n+1/2}(z) = \sqrt{\frac{\pi}{2z}} \frac{(2n-1)!!}{z^n}, \quad I_{n+1/2}(z) = \sqrt{\frac{2z}{\pi}} \frac{z^n}{(2n+1)!!}, \tag{33}$$

where $(2n-1)!! = 1 \cdot 3 \cdot \ldots \cdot (2n-1)$ (note that $(2n-1)!! = 1$ for $n = 0$). Therefore, for low $z \ll 1$

$$\frac{d}{dz}\left[\frac{I_{n+1/2}(z)}{\sqrt{z}}\right] = \sqrt{\frac{2}{\pi}} \frac{n z^{n-1}}{(2n+1)!!}, \quad \frac{d}{dz}\left[\frac{K_{n+1/2}(z)}{\sqrt{z}}\right] = -\sqrt{\frac{\pi}{2}} \frac{(n+1)(2n-1)!!}{z^{n+2}}. \tag{34}$$

According to boundary conditions (27) for small r_i the field should coincide with the field of the point charge $E_i = eq_i/r_i^2$, therefore, all A_n and C_n for all $n \geq 1$ should be equal to zero and the coefficients for $n = 0$ are determined by the relations:

$$A_0 = \sqrt{\tfrac{2}{\pi}}\, eq_1 k_D, \quad C_0 = \sqrt{\tfrac{2}{\pi}}\, eq_2 k_D. \tag{35}$$

It follows from (34) that

$$\lim_{a_i \to 0} \frac{d}{dr_i} \frac{I_{n+1/2}(\tilde{r}_i)}{\sqrt{\tilde{r}_i}} \bigg|_{r_i = a_i} = 0 \tag{36}$$

for all $n \geq 0$, therefore, the coefficients B_n, D_n are only determined by the external boundary conditions (28). It is seen from (34) that when $r_i \to 0$ the potential contains the additional term equal to $B_0\sqrt{\pi/2}$ and $D_0\sqrt{\pi/2}$ which should be subtracted from final expressions for the coefficients.

It follows from Eq. (36) and from boundary conditions (27) that the electric field of bulk charges connected with the i-th microparticle is zero in the location of this particle:

$$\lim_{a_i \to 0} E_{i,\varrho_i}(r_i = a_i) = -\lim_{a_i \to 0} \left(\frac{d\phi_i}{dr_i} + \frac{eq_i}{r_i^2} \right) \bigg|_{r = a_i} = 0. \tag{37}$$

Therefore, the i-th particle experiences only the force from charges induced by the other microparticle ($j = 3 - i$, $R = 2p$):

$$F_i = eq_i E_j \Big|_{\substack{r_j = R_{\rm int} \\ \theta_j = 0}} = -eq_i \left.\frac{d\phi_j}{dr_j}\right|_{\substack{r_j = R_{\rm int} \\ \theta_j = 0}} . \tag{38}$$

To use the boundary conditions (28) we have to reexpand solutions (31) and (32) by the Legendre polynomials with the pole in the point O. For this purpose let us use the Gegenbauer addition theorems [13] and decomposition theorem for the products $\tilde{r}_i^n P_n(\mu_i)$ ($\mu_i = \cos\theta_i$, $i = 1, 2$) [14] which are given in Appendix A. Finally, we get the following expression for the distribution of the potential of the first macroparticle in the spherical frame with the pole in the point O:

$$\begin{aligned} \phi_1(r,\mu) = {} & A_0 \sqrt{\tfrac{\pi}{2}} \sum_{m=0}^{\infty} (-1)^m (2m+1) \frac{K_{m+1/2}(u)}{u^{1/2}} \frac{I_{m+1/2}(v)}{v^{1/2}} P_m(\mu) \\ & + \sqrt{\tfrac{\pi}{2}} \sum_{n=0}^{\infty} B_n (2n-1)!! \left\{ \sum_{m=0}^{\infty} \sum_{k=0}^{n} \frac{n!\,(2n+2m+1)}{k!\,(n-k)!} \right. \\ & \left. \times \frac{I_{n+m+1/2}(\tilde{r})}{\tilde{r}^{1/2}} \frac{I_{n+m+1/2}(\tilde{p})}{\tilde{p}^{1/2}} \frac{1}{\tilde{p}^k \tilde{r}^{n-k}} P_k(\mu) C_m^{n+1/2}(\mu) \right\}. \end{aligned} \tag{39}$$

Here $\mu = \cos\theta$, $\tilde{p} = k_D p$, $C_m^{n+1/2}$ are the Gegenbauer polynomials [13], $u = \max(\tilde{r}, \tilde{p})$, $v = \min(\tilde{r}, \tilde{p})$. Similarly, for the second macroparticle:

$$\begin{aligned} \phi_2(r,\mu) = {} & C_0 \sqrt{\tfrac{\pi}{2}} \sum_{m=0}^{\infty} (2m+1) \frac{K_{m+1/2}(u)}{u^{1/2}} \frac{I_{m+1/2}(v)}{v^{1/2}} P_m(\mu) \\ & + \sqrt{\tfrac{\pi}{2}} \sum_{n=0}^{\infty} D_n (2n-1)!! \left\{ \sum_{m=0}^{\infty} \sum_{k=0}^{n} (-1)^{m+k} \frac{n!\,(2n+2m+1)}{k!\,(n-k)!} \right. \\ & \left. \times \frac{I_{n+m+1/2}(\tilde{r})}{\tilde{r}^{1/2}} \frac{I_{n+m+1/2}(\tilde{p})}{\tilde{p}^{1/2}} \frac{1}{\tilde{p}^k \tilde{r}^{n-k}} P_k(\mu) C_m^{n+1/2}(\mu) \right\}. \end{aligned} \tag{40}$$

The products of the Legendre and Gegenbauer polynomials can be expanded into the Legendre polynomials. As a result, we get the following potential distributions:

$$\phi_1(r,\mu) = \sum_{m=0}^{n_{\max}} \left[A_0 a_{0m}(\tilde{r}) + \sum_{k=0}^{n_{\max}} B_k b_{km}(\tilde{r}) \right] P_m(\mu), \tag{41}$$

$$\phi_2(r,\mu) = \sum_{m=0}^{n_{\max}} (-1)^m \left[C_0 a_{0m}(\tilde{r}) + \sum_{k=0}^{n_{\max}} D_k b_{km}(\tilde{r}) \right] P_m(\mu); \tag{42}$$

where a_{0m}, b_{km} are the expansion coefficients depending on coordinates of the considered point and interparticle distance. The explicit expressions of the coefficients for $m = 0, 1, \ldots, 5$ and $k = 0, 1, \ldots, 5$ are given in the Appendix B.

The external boundary conditions for the electric field and the potential (28) after a little algebra yield two independent equation systems for the variables $x_k = B_k + D_k$ and $y_k = B_k - D_k$, $k = 0, 1, \ldots, n_{\max}$ ($n_{\max}$ is an odd number):

$$\left.\begin{array}{l}\sum\limits_{k=0}^{n_{\max}} b_{km}x_k = -a_{0m}\left(A_0 + C_0\right), \\ \sum\limits_{k=0}^{n_{\max}} \beta_{km}x_k = -\alpha_{0m}\left(A_0 + C_0\right),\end{array}\right. \quad m = 0, 2, \ldots, n_{\max} - 1; \tag{43}$$

$$\left.\begin{array}{l}\sum\limits_{k=0}^{n_{\max}} b_{km}y_k = -a_{0m}\left(A_0 - C_0\right), \\ \sum\limits_{k=0}^{n_{\max}} \beta_{km}y_k = -\alpha_{0m}\left(A_0 - C_0\right),\end{array}\right. \quad m = 1, 3, \ldots, n_{\max}; \tag{44}$$

where

$$a_{0m} = a_{0m}\left(\tilde{r}\right)\big|_{\tilde{r}=\tilde{R}_b}, \quad b_{km} = b_{km}\left(\tilde{r}\right)\big|_{\tilde{r}=\tilde{R}_b}, \quad \alpha_{0m} = \left.\frac{\partial a_{0m}}{\partial \tilde{r}}\right|_{\tilde{r}=\tilde{R}_b}, \quad \beta_{km} = \left.\frac{\partial b_{km}}{\partial \tilde{r}}\right|_{\tilde{r}=\tilde{R}_b}.$$

The coefficients B_n, D_n from the solution of the systems (43) and 44) are easily found

$$B_n = \tfrac{1}{2}\left(x_n + y_n\right), \quad D_n = \tfrac{1}{2}\left(x_n - y_n\right).$$

Now we find the force of two microparticle interaction from (41) and (42)

$$F_1 = -eq_1k_D \sum_{m=0}^{n_{\max}} \left[C_0\alpha_{0m}\left(\tilde{p}\right) + \sum_{k=0}^{n_{\max}} D_k\beta_{km}\left(\tilde{p}\right)\right], \tag{45}$$

$$F_2 = -eq_2k_D \sum_{m=0}^{n_{\max}} \left[A_0\alpha_{0m}\left(\tilde{p}\right) + \sum_{k=0}^{n_{\max}} B_k\beta_{km}\left(\tilde{p}\right)\right]. \tag{46}$$

Figures 2 and 3 show the force dependencies on interparticle distance for two radii of the external boundary sphere: $R_b = 5/k_D$ and $R_b = 10/k_D$, calculated at $n_{\max} = 5$ for two identical charges. It is seen that taking account of terms up to $n_{\max} = 5$ provides adequate accuracy of the force definition up to $R_{\text{int}} = R_b$. The contribution of the multipole term $n_{\max} = 5$ becomes further more sufficient and it is necessary to take into account the higher multipole moments. Figure 2 shows the attraction of two like charged macroparticles at $R_{\text{int}} \gtrsim 4k_D^{-1}$. Figure 3 shows that this is the external boundary effect, since it disappears with double-sized computational cell, and the force is well described by the screened Debye potential.

Conclusion

This article shows that the attraction between like-charged microparticles in the equilibrium plasma within the Poisson-Boltzmann linearized theory applied to the finite size computation cell appears due to external boundary conditions. In the case of infinite cell all coefficients B_n, D_n $n = 0, 1, \ldots, \infty$ become zero and the potential distribution for each macroparticle according to Eqs. (31), (32) and (35) is described by the expressions:

$$\phi_1\left(r_i, \theta_i\right) = \sqrt{\tfrac{2}{\pi}}\, eq_ik_D \frac{K_{1/2}\left(\tilde{r}_i\right)}{\sqrt{\tilde{r}_i}}, \quad i = 1, 2. \tag{47}$$

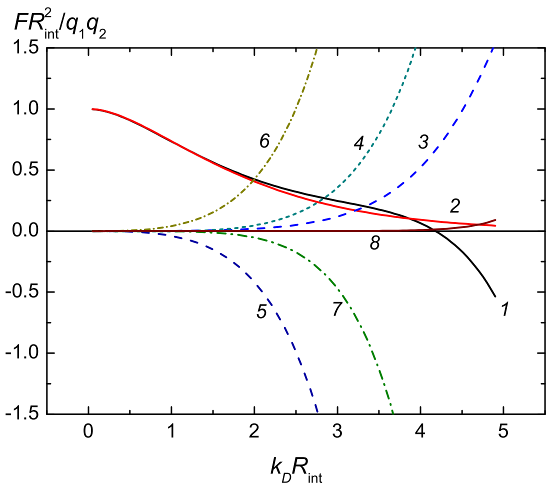

Figure 2. The interaction force of two point charges as a function of interparticle distance for $k_DR_b = 5$ and $q_1 = q_2$. Curve *1* is the total force, *2* is the Debye force connected with A_0, *3-8* are the partial forces due to multipole terms with $B_0 - B_5$.

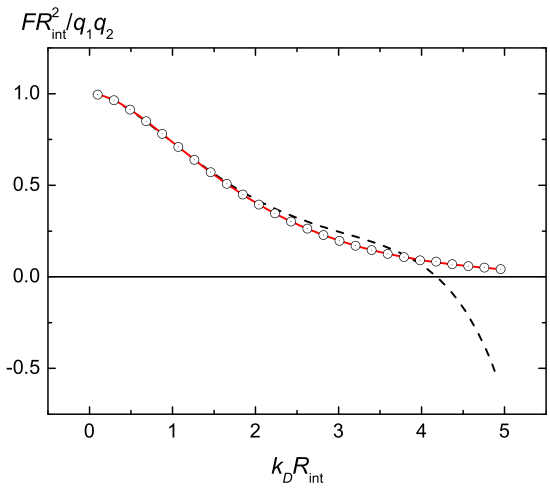

Figure 3. The interaction force of two point charges as a function of interparticle distance for $k_DR_b = 5$ and 10. The solid line corresponds to the Debye force, the dash line to the total force for $k_DR_b = 5$, symbols $\odot$ to the total force for $k_DR_b = 10$.

Substituting the explicit expression for the Bessel function $K_{1/2}$ [13], from (47) we obtain:

$$\phi_i\left(r_i, \theta_i\right) = \frac{eq_i}{r_i} e^{-k_D r_i}, \quad i = 1, 2. \tag{48}$$

From (38) and (48) we get

$$F_1 = F_2 = \frac{e^2 q_1 q_2}{R^2_{\text{int}}} \left(1 + k_D R_{\text{int}}\right) e^{-k_D R_{\text{int}}}. \tag{49}$$

So the attraction between two like-charged particles is clearly seen from Eq. (49) to be absent in the case of infinite cell.

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Appendix A. Addition theorems

Let us introduce the following notations: $(2n-1)!! = 1 \cdot 3 \cdot \ldots \cdot (2n-1)$, $\mu = \cos\theta$, $\mu_1 = \cos\theta_1$, $\mu_2 = \cos\theta_2$, $\tilde{r}_1 = k_D r_1$, $\tilde{r}_2 = k_D r_2$, $\tilde{p} = k_D p$, $u = \max\left(\tilde{r}, \tilde{p}\right)$, $v = \min\left(\tilde{r}, \tilde{p}\right)$. The Gegenbauer addition theorems ([13], p. 365) for angle geometry shown in figure 1 are as follows:

$$\frac{I_{n+1/2}\left(\tilde{r}_1\right)}{\tilde{r}_1{}^{n+1/2}} = (2n-1)!! \sqrt{\frac{\pi}{2}} \sum_{m=0}^{\infty} (2n+2m+1) \frac{I_{n+m+1/2}\left(\tilde{r}\right)}{\tilde{r}^{n+1/2}} \frac{I_{n+m+1/2}\left(\tilde{p}\right)}{\tilde{p}^{n+1/2}} C_m^{n+1/2}\left(\mu\right), \tag{A.1}$$

where $C_m^{n+1/2}$ are Gegenbauer polynomials [13],

$$\frac{K_{1/2}\left(\tilde{r}_1\right)}{\tilde{r}_1{}^{1/2}} = \sqrt{\frac{\pi}{2}} \sum_{m=0}^{\infty} (-1)^m (2m+1) \frac{K_{m+1/2}\left(u\right)}{u^{1/2}} \frac{I_{m+1/2}\left(v\right)}{v^{1/2}} P_m\left(\mu\right); \tag{A.2}$$

$$\frac{I_{n+1/2}\left(\tilde{r_2}\right)}{\tilde{r_2}^{n+1/2}} = (2n-1)!!\sqrt{\tfrac{\pi}{2}} \times \sum_{m=0}^{\infty} (-1)^m (2n+2m+1) \frac{I_{n+m+1/2}\left(\tilde{r}\right)}{\tilde{r}^{n+1/2}} \frac{I_{n+m+1/2}\left(\tilde{p}\right)}{\tilde{p}^{n+1/2}} C_m^{n+1/2}(\mu), \quad \text{(A.3)}$$

$$\frac{K_{1/2}\left(\tilde{r_2}\right)}{\tilde{r_2}^{1/2}} = \sqrt{\tfrac{\pi}{2}} \sum_{m=0}^{\infty} (2m+1) \frac{K_{m+1/2}(u)}{u^{1/2}} \frac{I_{m+1/2}(v)}{v^{1/2}} P_m(\mu). \quad \text{(A.4)}$$

The addition formulas for vectors and angles in figure 1 are as follows [14]:

$$\tilde{r}_1^n P_n(\mu_1) = \sum_{k=0}^{n} \frac{n!}{k!\,(n-k)!} \tilde{r}^k \tilde{p}^{n-k} P_k(\mu), \quad \text{(A.5)}$$

$$\tilde{r}_2^n P_n(\mu_2) = \sum_{k=0}^{n} (-1)^k \frac{n!}{k!\,(n-k)!} \tilde{r}^k \tilde{p}^{n-k} P_k(\mu). \quad \text{(A.6)}$$

Appendix B. The coefficients of potential and electric field expansion in terms of Legendre polynomials with the pole at the point O

For convenience let us introduce the following functions:

$$\begin{aligned} \Phi_{m+1/2}\left(\tilde{r},\tilde{p}\right) &= \sqrt{\tfrac{1}{2}\pi}\,(2m+1) \frac{K_{m+1/2}\left(\tilde{r}\right)}{\tilde{r}^{1/2}} \frac{I_{m+1/2}\left(\tilde{p}\right)}{\tilde{p}^{1/2}}, \\ \Psi_{m+1/2}\left(\tilde{r},\tilde{p}\right) &= \sqrt{\tfrac{1}{2}\pi}\,(2m+1) \frac{I_{m+1/2}\left(\tilde{r}\right)}{\tilde{r}^{1/2}} \frac{I_{m+1/2}\left(\tilde{p}\right)}{\tilde{p}^{1/2}}. \end{aligned} \quad \text{(B.1)}$$

Then the coefficients of potential expansion in terms of Legendre polynomials with the pole at the point O take the form:

$$a_{0m}\left(\tilde{r}\right) = (-1)^m \Phi_{m+1/2}, \quad b_{0m}\left(\tilde{r}\right) = \Psi_{m+1/2} - \delta_{m0}\sqrt{\pi/2}, \quad m = 0, 1, \ldots, n_{\max}; \quad \text{(B.2)}$$

$$\begin{aligned} b_{10}\left(\tilde{r}\right) &= \frac{\Psi_{3/2}}{\tilde{r}} + \frac{\Psi_{5/2}}{\tilde{p}} + \frac{\Psi_{7/2}}{\tilde{r}} + \frac{\Psi_{9/2}}{\tilde{p}} + \frac{\Psi_{11/2}}{\tilde{r}}, \\ b_{11}\left(\tilde{r}\right) &= \frac{\Psi_{3/2}}{\tilde{p}} + \frac{3\Psi_{5/2}}{\tilde{r}} + \frac{3\Psi_{7/2}}{\tilde{p}} + \frac{3\Psi_{9/2}}{\tilde{r}} + \frac{3\Psi_{11/2}}{\tilde{p}}, \\ b_{12}\left(\tilde{r}\right) &= \frac{2\Psi_{5/2}}{\tilde{p}} + \frac{5\Psi_{7/2}}{\tilde{r}} + \frac{5\Psi_{9/2}}{\tilde{p}} + \frac{5\Psi_{11/2}}{\tilde{r}}, \quad b_{13}\left(\tilde{r}\right) = \frac{3\Psi_{7/2}}{\tilde{p}} + \frac{7\Psi_{9/2}}{\tilde{r}} + \frac{7\Psi_{11/2}}{\tilde{p}}, \\ b_{14}\left(\tilde{r}\right) &= \frac{4\Psi_{9/2}}{\tilde{p}} + \frac{9\Psi_{11/2}}{\tilde{r}}, \quad b_{15}\left(\tilde{r}\right) = \frac{5\Psi_{11/2}}{\tilde{p}}; \end{aligned} \quad \text{(B.3)}$$

$$\begin{aligned} b_{20}\left(\tilde{r}\right) &= \frac{3\Psi_{5/2}}{\tilde{r}^2} + \frac{10\Psi_{7/2}}{\tilde{p}\tilde{r}} + \frac{10\Psi_{9/2}}{\tilde{r}^2} + \frac{7\Psi_{9/2}}{\tilde{p}^2} + \frac{28\Psi_{11/2}}{\tilde{p}\tilde{r}}, \\ b_{21}\left(\tilde{r}\right) &= \frac{6\Psi_{5/2}}{\tilde{p}\tilde{r}} + \frac{15\Psi_{7/2}}{\tilde{r}^2} + \frac{6\Psi_{7/2}}{\tilde{p}^2} + \frac{48\Psi_{9/2}}{\tilde{p}\tilde{r}} + \frac{42\Psi_{11/2}}{\tilde{r}^2} + \frac{33\Psi_{11/2}}{\tilde{p}^2} \\ b_{22}\left(\tilde{r}\right) &= \frac{3\Psi_{5/2}}{\tilde{p}^2} + \frac{20\Psi_{7/2}}{\tilde{p}\tilde{r}} + \frac{35\Psi_{9/2}}{\tilde{r}^2} + \frac{20\Psi_{9/2}}{\tilde{p}^2} + \frac{110\Psi_{11/2}}{\tilde{p}\tilde{r}}, \\ b_{23}\left(\tilde{r}\right) &= \frac{9\Psi_{7/2}}{\tilde{p}^2} + \frac{42\Psi_{9/2}}{\tilde{p}\tilde{r}} + \frac{63\Psi_{11/2}}{\tilde{r}^2} + \frac{42\Psi_{11/2}}{\tilde{p}^2}, \\ b_{24}\left(\tilde{r}\right) &= \frac{18\Psi_{9/2}}{\tilde{p}^2} + \frac{24\Psi_{11/2}}{\tilde{p}\tilde{r}}, \quad b_{25}\left(\tilde{r}\right) = \frac{30\Psi_{11/2}}{\tilde{p}^2}; \end{aligned} \quad \text{(B.4)}$$

$$\begin{aligned}
b_{30}\left(\tilde{r}\right) &= \frac{15\Psi_{7/2}}{\tilde{r}^3} + \frac{105\Psi_{9/2}}{\tilde{p}\tilde{r}^2} + \frac{105\Psi_{11/2}}{\tilde{r}^3} + \frac{189\Psi_{11/2}}{\tilde{p}^2\tilde{r}}, \\
b_{31}\left(\tilde{r}\right) &= \frac{45\Psi_{7/2}}{\tilde{p}\tilde{r}^2} + \frac{105\Psi_{9/2}}{\tilde{r}^3} + \frac{126\Psi_{9/2}}{\tilde{p}^2\tilde{r}} + \frac{693\Psi_{11/2}}{\tilde{p}\tilde{r}^2} + \frac{81\Psi_{11/2}}{\tilde{p}^3}, \\
b_{32}\left(\tilde{r}\right) &= \frac{45\Psi_{7/2}}{\tilde{p}^2\tilde{r}} + \frac{210\Psi_{9/2}}{\tilde{p}\tilde{r}^2} + \frac{45\Psi_{9/2}}{\tilde{p}^3} + \frac{315\Psi_{11/2}}{\tilde{r}^3} + \frac{585\Psi_{11/2}}{\tilde{p}^2\tilde{r}}, \\
b_{33}\left(\tilde{r}\right) &= \frac{15\Psi_{7/2}}{\tilde{p}^3} + \frac{189\Psi_{9/2}}{\tilde{p}^2 r} + \frac{567\Psi_{11/2}}{\tilde{p} r^2} + \frac{189\Psi_{11/2}}{\tilde{p}^3}, \\
b_{34}\left(\tilde{r}\right) &= \frac{60\Psi_{9/2}}{\tilde{p}^3} + \frac{486\Psi_{11/2}}{\tilde{p}^2 r}, \quad b_{35}\left(\tilde{r}\right) = \frac{150\Psi_{11/2}}{\tilde{p}^3};
\end{aligned} \tag{B.5}$$

$$\begin{aligned}
b_{40}\left(\tilde{r}\right) &= \frac{105\Psi_{9/2}}{\tilde{r}^4} + \frac{1260\Psi_{11/2}}{\tilde{p}\tilde{r}^3}, \quad b_{41}\left(\tilde{r}\right) = \frac{420\Psi_{9/2}}{\tilde{p} r^3} + \frac{945\Psi_{11/2}}{r^4} + \frac{2268\Psi_{11/2}}{\tilde{p}^2 r^2}, \\
b_{42}\left(\tilde{r}\right) &= \frac{630\Psi_{9/2}}{\tilde{p}^2 r^2} + \frac{2520\Psi_{11/2}}{\tilde{p} r^3} + \frac{1620\Psi_{11/2}}{\tilde{p}^3\tilde{r}}, \\
b_{43}\left(\tilde{r}\right) &= \frac{420\Psi_{9/2}}{\tilde{p}^3\tilde{r}} + \frac{3402\Psi_{11/2}}{\tilde{p}^2 r^2} + \frac{420\Psi_{11/2}}{\tilde{p}^4}, \\
b_{44}\left(\tilde{r}\right) &= \frac{105\Psi_{9/2}}{\tilde{p}^4} + \frac{2160\Psi_{11/2}}{\tilde{p}^3\tilde{R}}, \quad b_{45}\left(\tilde{r}\right) = \frac{525\Psi_{11/2}}{\tilde{p}^4};
\end{aligned} \tag{B.6}$$

$$\begin{aligned}
b_{50}\left(\tilde{r}\right) &= \frac{945\Psi_{11/2}}{r^5}, \quad b_{51}\left(\tilde{r}\right) = \frac{4725\Psi_{11/2}}{\tilde{p} r^4}, \quad b_{52}\left(\tilde{r}\right) = \frac{9450\Psi_{11/2}}{\tilde{p}^2 r^3}, \\
b_{53}\left(\tilde{r}\right) &= \frac{9450\Psi_{11/2}}{\tilde{p}^3 r^2}, \quad b_{54}\left(\tilde{r}\right) = \frac{4725\Psi_{11/2}}{\tilde{p}^4\tilde{r}}, \quad b_{55}\left(\tilde{r}\right) = \frac{945\Psi_{11/2}}{\tilde{p}^5}.
\end{aligned} \tag{B.7}$$

The coefficients α_{0m} and β_{km} can be easily calculated from the expressions for a_{0m} and b_{km} using the follow formulae:

$$\begin{aligned}
\frac{\partial}{\partial \tilde{r}}\left(\frac{\Phi_{m+1/2}}{\tilde{r}^k}\right) &= -\frac{\Phi^1_{m+1/2}}{\tilde{r}^k} + \frac{(m-k)\,\Phi_{m+1/2}}{\tilde{r}^{k+1}} \\
\frac{\partial}{\partial \tilde{r}}\left(\frac{\Psi_{m+1/2}}{\tilde{r}^k}\right) &= \frac{\Psi^1_{m+1/2}}{\tilde{r}^k} + \frac{(m-k)\,\Psi_{m+1/2}}{\tilde{r}^{k+1}}
\end{aligned} \tag{B.8}$$

where we introduce the new functions:

$$\begin{aligned}
\Phi^1_{m+1/2}\left(\tilde{r},\tilde{p}\right) &= \sqrt{\tfrac{1}{2}\pi}\,(2m+1)\,\frac{K_{m+3/2}\left(\tilde{r}\right)}{\tilde{r}^{1/2}}\,\frac{I_{m+1/2}\left(\tilde{p}\right)}{\tilde{p}^{1/2}}, \\
\Psi^1_{m+1/2}\left(\tilde{r},\tilde{p}\right) &= \sqrt{\tfrac{1}{2}\pi}\,(2m+1)\,\frac{I_{m+3/2}\left(\tilde{r}\right)}{\tilde{r}^{1/2}}\,\frac{I_{m+1/2}\left(\tilde{p}\right)}{\tilde{p}^{1/2}}.
\end{aligned} \tag{B.9}$$

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