

Interaction in equilibrium plasmas of charged macroparticles located in nodes of cubic lattices

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Abstract. Interaction of two charged pointlike macroparticles located at nodes of simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc) lattices in an equilibrium plasma is studied within the linearized Poisson–Boltzmann model. It is shown that the boundary shape has a strong influence on the electrostatic interaction between two macroparticles, which switches from repulsion at small interparticle distances to attraction as it approaches the half-length of a computational cell. It is found that in a case of dust particles arranged in the nodes of the sc, bcc and fcc lattices, the electrostatic force acting on them is equal to zero and the nature of the interaction changes from repulsion to attraction; hence, the infinite sc, bcc and fcc lattices of charged dust particles are thermodynamically stable at rather low temperatures.

1. Introduction

In the framework of the Poisson–Boltzmann model using the Cassini coordinates, Gundienkov and Yakovlenko [1] numerically studied the interaction of two macroparticles placed in a finite size cell with a outer boundary of a Cassini oval shape. The electric force exerted on a macroparticle by the other macroparticle was determined using the Maxwell stress tensor. It was found that under certain conditions there is an effect of attraction between two similarly charged macroparticles at distances close to the half Debye radius. It was shown [2–7] that within the Poisson–Boltzmann model in an infinite cell there is no attraction between similarly charged point particles (see, also [8–10]). In [7,11], the electrostatic interaction of two macroparticles was considered for calculation cells of spherical, cylindrical and ellipsoidal forms and the attraction between similarly charged macroparticles was found at interparticle distances close to the Debye radius. The present paper is devoted to studying the influence of external boundary shapes on the interaction of two charged pointlike particles in an equilibrium plasma within the Debye–Hückel approximation [12]. Outer boundary shapes corresponding to two adjacent to each other Seitz–Wigner cells of the simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc) lattices are considered.

2. Solution of the Poisson equation for axially symmetric outer boundary

Definition of an axially symmetric shape of the outer boundary using two adjoined Wigner–Seitz (WS) cells for the problem of interaction of two pointlike macroparticles is shown in figure 1 (definition of the WS cell is in [13,14]). All physical quantities including the electric field potential are symmetrical about the planes shown in figure 1 by dashed lines, therefore the



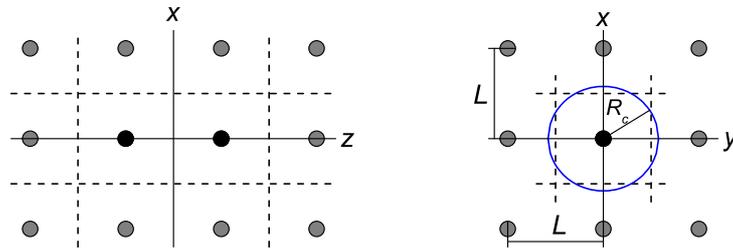


Figure 1. The Wigner–Zeits cell and the computational cell for the problem of electrostatic interaction of two macroparticles in a crystal with the simple cubic lattice ($R_c = L/\sqrt{\pi}$). The dashed lines indicate symmetry planes on which the normal component of the electric field strength is equal to zero.

normal derivative of the electric field potential on these planes is equal to zero. In a case of macroparticles arranged in nodes of the sc lattice, the WS cell is a cube of edge length a which equals the distance between the nearest neighbor macroparticles: $L = a$; the WS cell volume $V_{sc} = L^3$. The WS cell for the fcc lattice is a rhombic dodecahedron, which has 12 faces of the rhombic form with the ratio of diagonals equal to $1 : \sqrt{2}$ and with side $b = \sqrt{3}a/4$. Here and further a is the cube edge length of the unit cell of the sc, fcc and bcc lattices. In the case of the fcc lattice the distance between the nearest neighbor macroparticles is defined by $L = a/\sqrt{2}$ and the WS volume $V_{fcc} = L^3/\sqrt{2}$. The WS cell of the bcc lattice is a truncated octahedron produced by 6 quadratic faces and 8 faces in the form of regular hexagons. The sides of the squares and the regular hexagons are the same and are determined from $b = a/\sqrt{8}$, the distance between the nearest neighbor macroparticles given by $L = a\sqrt{3}/2$ and the WS volume $V_{bcc} = 4(L/\sqrt{3})^3$.

The Wigner–Seitz method, in which the WS cell is replaced by a sphere of the same volume, is widely used in the solid state physics [13]. For the problem under consideration, it is required to consider two adjacent to each other WS cells of two nearest neighbor macroparticles. Therefore, to simplify the problem on the analogy of the Wigner–Seitz method we select the axially symmetric shape of the computational cell based on the condition that in any cross section by a plane perpendicular to the axis z the area of the cross sections of the computational cell, $\pi R_z^2(z)$, and of the two nearest neighbor WS cells, $S(z)$, are equal to each other:

$$R_z(z) = \sqrt{S(z)/\pi}.$$

The length of the radius-vector to the outer boundary point in the spherical coordinate system with the origin at the point O (see figure 2) is defined by $R_b = \sqrt{R_z^2 + z^2}$. This is the implicit relation which determines the function $R_b(\mu)$. For the sc lattice, the computational cell is a cylinder with the radius $R_c = L/\sqrt{\pi}$ and the height equal to $2L$, for the bcc and fcc lattices the computational cell is bounded by more complex surfaces of revolution (see figure 2). The geometry of the interaction of two macroparticles in an equilibrium dusty plasma and dependencies of the radius of cross sections by (x, y) -plane of the computational cell at z are shown in figure 2 for the sc, bcc and fcc lattices and for the spheroid with the volume equal to $2L^3$.

In this paper we consider the interaction of two macroparticles of small radii: $k_D a_1 \ll 1$, $k_D a_2 \ll 1$, where a_1 , a_2 are their radii. We define the self-consistent potential of charged macroparticles and equilibrium plasma using the linearized Poisson–Boltzmann equation [12]

$$\Delta\phi + k_D^2\phi = 0, \quad (1)$$

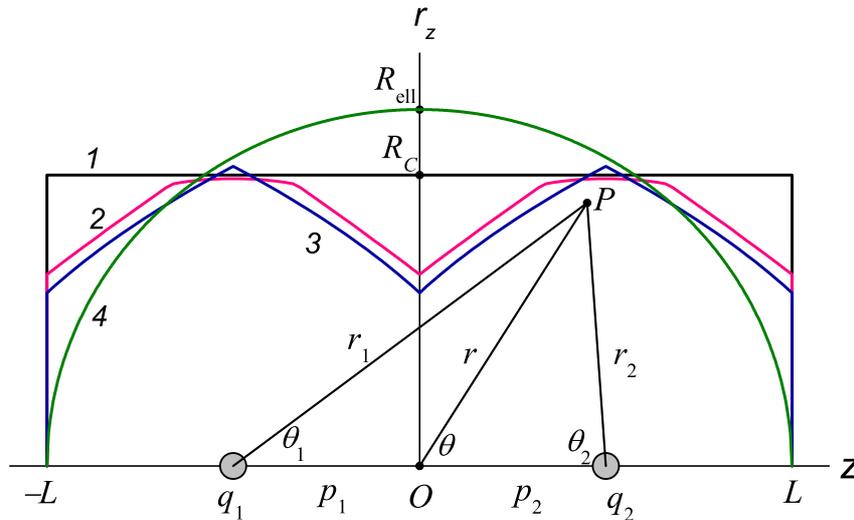


Figure 2. Geometry of the problem of the two-particle interaction with the outer boundary in the shape of a cylinder with radius R_c (1) for the sc lattice, axisymmetric surfaces with the varied radius $R_z(z)$ of cross sections for bcc (2) and fcc lattices (3), and a spheroid (4). Here, $r_z = \sqrt{x^2 + y^2}$, $R_c = L/\sqrt{\pi}$, $R_{\text{ell}} = L/\sqrt{\alpha}$, $\alpha = \frac{2}{3}\pi$, $p_1 + p_2 = R$, R is the interparticle distance, q_1 and q_2 are the charges of macroparticles in elementary charges, P is the field point.

where k_D is the inverse Debye radius:

$$k_D^2 = 4\pi e^2 \left(\frac{n_{i0}}{T_i} + \frac{n_{e0}}{T_e} \right),$$

n_{e0} and n_{i0} are the number densities of electrons and ions, respectively, in the unperturbed plasma, and T_e , T_i are their temperatures in energetic units.

We apply the following boundary conditions ($i = 1, 2$):

$$\left. \frac{\partial \phi_i(r_i, \theta_i)}{\partial r_i} \right|_{r_i=a_i} = -\frac{eq_i}{a_i^2}, \tag{2}$$

and the condition on the outer boundary, which is due to the symmetry of the problem under consideration:

$$E_n(r, \theta)|_{r=R_b(\theta)} = 0, \tag{3}$$

where E_n is the normal component of the electric field strength on the outer boundary defined by the equation $r = R_b(\theta)$. Condition (3) provides the quasi-neutrality of the computational cell. From conditions (2), it is seen that the electric field potential is defined up to a constant which is physically meaningless (for more details see [7]).

The problem is linear, so the solution of equation (1) can be found as a superposition of three terms:

$$\phi(r, \theta) = \phi_1(r_1) + \phi_2(r_2) + \phi_3(r, \theta), \tag{4}$$

where ϕ_1 is the screened potential of the first macroparticle in infinite plasma, which will ensure the fulfillment of condition (2) for $i = 1$; ϕ_2 is the screened potential of the second macroparticle in infinite plasma, which will ensure the fulfillment of condition (2) for $i = 2$; ϕ_3 is the potential of additional bulk charges, which will ensure the fulfillment of condition (3).

Considering the cylindrical symmetry of problem (1) with boundary conditions (2) and (3), the solutions for potential components (4) can be written in the following forms [7, 15]:

$$\begin{aligned} \phi_i(r_i) &= A_i \frac{K_{1/2}(k_D r_i)}{\sqrt{k_D r_i}}, \quad i = 1, 2; \\ \phi_3(r, \mu) &= \sum_{n=0}^{\infty} C_n \frac{I_{n+1/2}(k_D r)}{\sqrt{k_D r}} P_n(\mu), \end{aligned} \tag{5}$$

where $I_{n+1/2}$, $K_{n+1/2}$ are the modified Bessel functions of the first and third kind, respectively [16], and P_n are the Legendre polynomials. The coefficients A_1 and A_2 according to (2) are defined by the following relations [7]:

$$A_1 = \sqrt{\frac{2}{\pi}} e q_1 k_D, \quad A_2 = \sqrt{\frac{2}{\pi}} e q_2 k_D. \tag{6}$$

Boundary condition (3) can be rewritten in the form:

$$(\mathbf{n} \cdot \nabla \phi)|_{r=R_b} = 0, \tag{7}$$

where \mathbf{n} is the normal to the outer boundary. For the axisymmetric outer boundary, the normal is given by

$$\mathbf{n} = n_r \mathbf{e}_r + n_\theta \sin \theta \mathbf{e}_\theta; \tag{8}$$

where \mathbf{e}_r , \mathbf{e}_θ are the orthogonal unit vectors of the spherical coordinate system (see figure 2) and

$$n_r = \frac{R_b}{\sqrt{R_b^2 + (\partial R_b / \partial \theta)^2}}, \quad n_\theta = \frac{\partial R_b / \partial \mu}{\sqrt{R_b^2 + (\partial R_b / \partial \theta)^2}},$$

$\mu = \cos \theta$. Let us expand the boundary condition (7) in Legendre polynomials

$$\sum_{k=0}^{\infty} D_k P_k(\mu) = 0, \quad k = 0, 1, 2, \dots, \tag{9}$$

where the expansion coefficients D_k are determined from

$$D_k = \frac{2k+1}{2} \int_{-1}^1 (\mathbf{n} \cdot \nabla \phi)|_{r=R_b} P_k(\mu) d\mu. \tag{10}$$

From equation (9), owing to the linear independency of the Legendre polynomials, it follows that $D_k = 0$ for all $k = 0, 1, 2, \dots$. Hence, from equations (8) and (10), we obtain

$$D_k = \frac{2k+1}{2} \int_{-1}^1 \left(n_r \frac{\partial \phi}{\partial r} \Big|_{r=R_b} - n_\theta \frac{1-\mu^2}{R_b} \frac{\partial \phi}{\partial \mu} \Big|_{r=R_b} \right) \times P_k(\mu) d\mu \equiv 0, \quad k = 0, 1, 2, \dots \tag{11}$$

Let us introduce the definitions ($i = 1, 2$):

$$\begin{aligned} E_{i,r} &= -\frac{\partial \phi_i}{\partial r} = e k_D^2 q_i \frac{(1 + \tilde{r}_i)}{\tilde{r}_i^3} e^{-\tilde{r}_i} [\tilde{r} - (-1)^i \tilde{p}_i \mu], \\ E_{i,\theta} &= -\frac{1}{r} \frac{\partial \phi_i}{\partial \theta} = (-1)^i e k_D^2 q_i \frac{(1 + \tilde{r}_i)}{\tilde{r}_i^3} e^{-\tilde{r}_i} \tilde{p}_i \sin \theta. \end{aligned}$$

Here q_1 and q_2 are the charges of macroparticles in elementary charges, $\tilde{r} = k_D r$, $\tilde{r}_1 = k_D r_1$, $\tilde{p}_1 = k_D p_1$, $\tilde{r}_2 = k_D r_2$, $\tilde{p}_2 = k_D p_2$, $r_1 = \sqrt{r^2 + p_1^2 + 2p_1 r \mu}$, and $r_2 = \sqrt{r^2 + p_2^2 - 2p_2 r \mu}$. For the components of the field strength at the outer boundary, we now have:

$$E_r|_{r=R_b} = E_{1,r}|_{r=R_b} + E_{2,r}|_{r=R_b} - ek_D^2 \sum_{n=0}^{\infty} C_n P_n(\mu) \frac{\partial}{\partial \tilde{R}_b} \left[\frac{I_{n+1/2}(\tilde{R}_b)}{\tilde{R}_b^{1/2}} \right], \quad (12)$$

$$E_\theta|_{r=R_b} = E_{1,\theta}|_{r=R_b} + E_{2,\theta}|_{r=R_b} + ek_D^2 \sum_{n=0}^{\infty} C_n \frac{I_{n+1/2}(\tilde{R}_b)}{\tilde{R}_b^{3/2}} (1 - \mu^2)^{1/2} \frac{\partial P_n(\mu)}{\partial \mu}.$$

We introduce the following definitions:

$$I_{kn}^r = \frac{2k+1}{2} \int_{-1}^1 n_r P_k P_n \frac{\partial}{\partial \tilde{R}_b} \left[\frac{I_{n+1/2}(\tilde{R}_b)}{\tilde{R}_b^{1/2}} \right] d\mu, \quad (13)$$

$$I_{kn}^\mu = -\frac{2k+1}{2} \int_{-1}^1 n (P_{n-1} - \mu P_n) P_k \frac{n_\theta}{\tilde{R}_b} \frac{I_{n+1/2}(\tilde{R}_b)}{\tilde{R}_b^{1/2}} d\mu; \quad (14)$$

$$I_k^{ir} = \frac{2k+1}{2} \int_{-1}^1 \frac{(1 + \tilde{r}_i)}{\tilde{r}_i^3} e^{-\tilde{r}_i} \Big|_{r=R_b} n_r \left[\tilde{R}_b - (-1)^i \tilde{p}_i \mu \right] P_k d\mu, \quad (15)$$

$$I_k^{i\mu} = (-1)^i \frac{2k+1}{2} \int_{-1}^1 \frac{(1 + \tilde{r}_i)}{\tilde{r}_i^3} e^{-\tilde{r}_i} \Big|_{r=R_b} \tilde{p}_i n_\theta (1 - \mu^2) P_k d\mu. \quad (16)$$

Using these definitions from equation (11) for the potential expansion coefficients C_n we obtain the system of equations:

$$\sum_{n=0}^{\infty} a_{kn} C_n = b_k, \quad k = 0, 1, 2, \dots, \quad (17)$$

where $a_{kn} = (I_{kn}^r + I_{kn}^\mu)$ and $b_k = q_1 (I_k^{1r} + I_k^{1\mu}) + q_2 (I_k^{2r} + I_k^{2\mu})$.

If the size of the macroparticles can be neglected, the force acting on any chosen macroparticle is determined by the electric field strength at the point of the location of this macroparticle ($i = 1, 2, j = 3 - i$):

$$F_{ij} = -eq_i \left[\frac{\partial \phi_j}{\partial r_j} \Big|_{r_j=R} + \frac{\partial \phi_3(r, \mu)}{\partial r} \Big|_{\substack{r=p_i \\ \mu=(-1)^i}} \right]. \quad (18)$$

Here, we consider that according to boundary conditions (2), the residual electric field of the i -th ($i = 1, 2$) macroparticle after the subtraction of its Coulomb field at the point of its location is equal to zero.

3. Numerical simulation results and discussion

Numerical simulations are performed for macroparticles with the equal charges $q_1 = q_2$ and for $p_1 = p_2 = \frac{1}{2}R$ (here R is the interparticle distance). Figure 3 presents the two-dimensional distributions of the total potential $\phi(\tilde{r}_z, \tilde{z})$ and the potential of bulk charges $\phi_3(\tilde{r}_z, \tilde{z})$ in the computational cell for the bcc lattice. Here $\tilde{r}_z = k_D r_z$, $\tilde{z} = k_D z$.

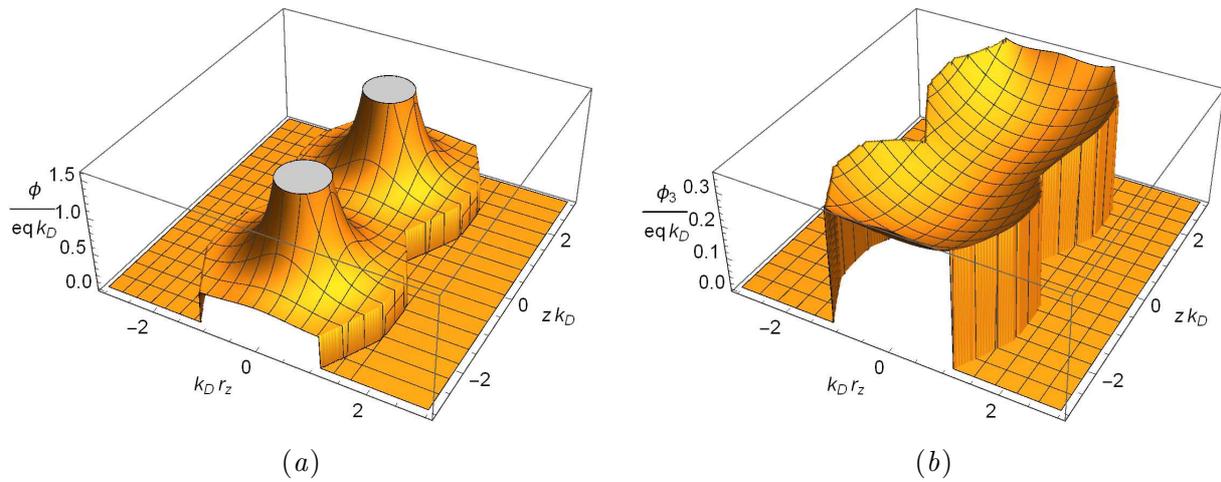


Figure 3. Two-dimensional distributions of the total potential ϕ (a) and the potential of bulk charges ϕ_3 (b) in the computational cell for the bcc lattice at $k_D L = 3$, $R_c = L/\sqrt{\pi}$, $R = L$, $n_{\max} = 50$.

From figure 3a, one can see that the total potential reaches extreme values (the minimum for the positive charges q_1 and q_2) only on the outer boundary and inside the cell there is only a saddle point at the origin point O . From figure 3b, it is evident that an additional bulk charge for positive charges $q_1 = q_2 > 0$ is negative (the additional charge density is determined from $\rho_3 = -k_D^2 \phi_3 / 4\pi$), and its density increases as we approach the computational cell boundary.

Figure 4 presents the dependence of the interaction force of two point macroparticles on the interparticle distance for the case of the computational cell of the cylindrical form with different half-lengths L . We see that the interaction force at small interparticle distances, $k_D R \ll 1$, is close to the Debye force defined by the equation

$$F_D = \frac{e^2 q_1 q_2}{R^2} (1 + k_D R) \exp(-k_D R). \quad (19)$$

It is notable that the interaction force is repulsive at intermediate distances $R \sim \frac{1}{2}L$, exceeds the Debye force and passes through the maximum, the height of which decreases with increasing the computational cell length.

The interaction force dependencies for the case of the computational cell in the spheroid form with the volume equal to two volumes of the WS cell of the sc lattice are presented in figure 5. One can see that the interaction force is less than the Debye force at all interparticle distances and the repulsion between the macroparticles changes to attraction at distances $R \approx \frac{4}{5}L$. Note that at $R = L$, the attraction between the macroparticles in the spheroid is strong.

From figure 4 we see that the interaction force between the macroparticles located in the nodes of a simple cubic lattice (i.e., when $R = L$) is equal to zero. The interaction force at this point passes through zero, changing the nature of the interaction from repulsion to attraction. Thus, the electrostatic interaction potential has a minimum at $R = L$. This suggests that the system of macroparticles located at the nodes of the sc lattice in the equilibrium plasma should be mechanically stable, i.e. thermodynamically stable at sufficiently low temperatures.

Figure 6 shows the interaction force dependence at different radii of the cylindrical cell (in this case, the volume of the computational cell is certainly different from that of two SW cells unless the cylinder radius is equal to $L/\sqrt{\pi}$). It is clear that both the increase and the decrease in R_c hardly change the positions of equilibrium points of the macroparticles. If the conditions $a_1 \ll L$ and $a_2 \ll L$ are fulfilled, considering the finite size of the macroparticles does not

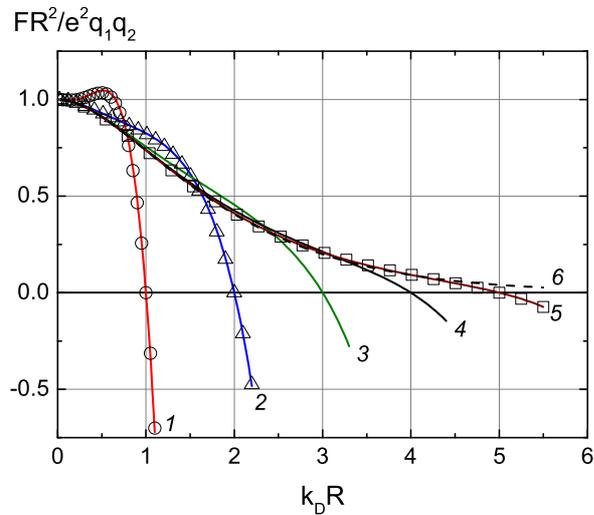


Figure 4. Interaction force as a function of the interparticle distance R for $R_c = L/\sqrt{\pi}$, $n_{\max} = 50$ at different lengths of the sc lattice: curve 1 is for $k_D L = 1$, 2 for $k_D L = 2$, 3 for $k_D L = 3$, 4 for $k_D L = 4$, and 5 for $k_D L = 5$; 6 is the Debye dependence and symbols are data calculated from (20).

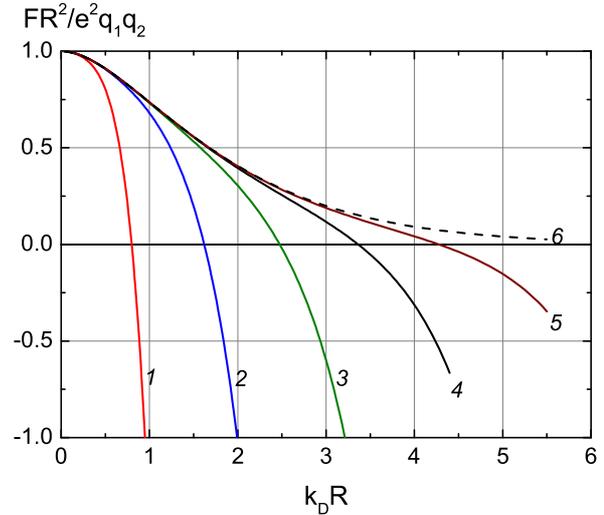


Figure 5. The interaction force as a function of R for the computational cell in the form of the spheroid (ellipsoid of revolution with $s = 1$), $\alpha = 2\pi/3$. Curve 1 is for $k_D L = 1$, 2 for $k_D L = 2$, 3 for $k_D L = 3$, 4 for $k_D L = 4$, and 5 for $k_D L = 5$; 6 is the Debye dependence.

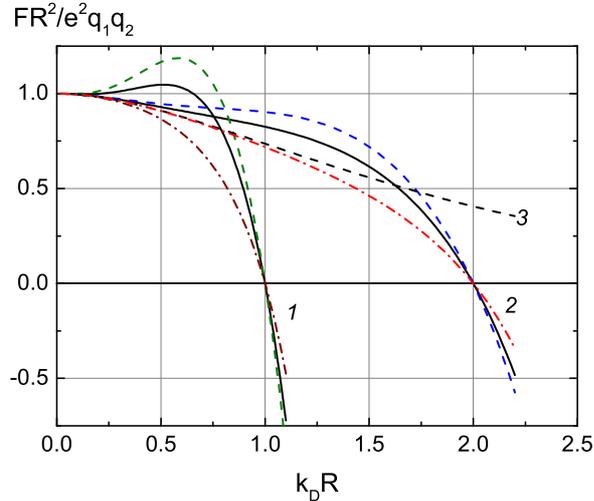


Figure 6. Interaction force vs R at different R_c for $k_D L = 1$ (curves 1) and $k_D L = 2$ (curves 2) for $n_{\max} = 50$. The solid curves are calculated for $R_c = L/\sqrt{\pi}$, the dashed lines for $R_c = L/2$ and the dot-and-dash lines are for $R_c = L$, 3 is the Debye dependence.

practically change the interaction force at distances $R \sim L$, because the size of macroparticles is affected only at distances $R \sim \min(a_1, a_2)$ (see [17–20] and the literature cited in them).

The interaction force dependencies for the computational cells of the sc, bcc and scc lattices are presented in figure 7 at $k_D L = 2$ and $k_D L = 4$. In insertions in this figure, regions of the sign change of the interaction force are shown in an enlarged scale.

Considering the symmetry of the problem under consideration in the case of location of the macroparticles at the nodes of the sc, fcc and bcc lattices, it is evident that the interaction force becomes equal to zero at $R = L$. The problem considered in the present paper corresponds to the problem of interaction of an ensemble of macroparticles arranged so that a change in the interparticle distance between two selected particles does not change the shape of the

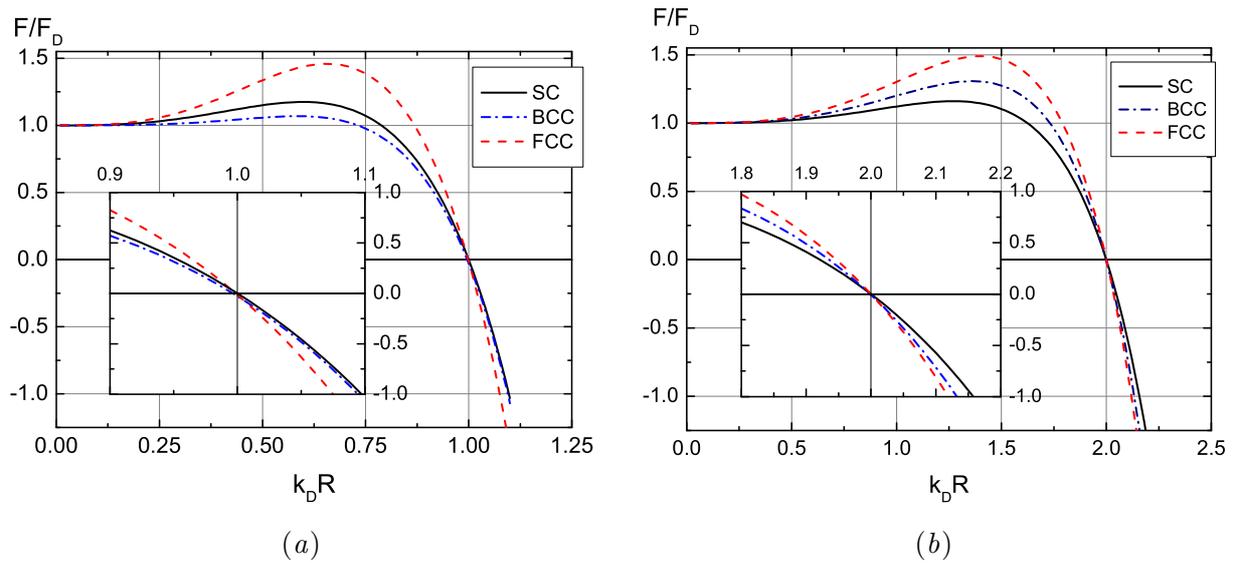


Figure 7. The interaction force as a function R for the computational cells of sc, bcc and sc lattices at $k_D L = 2$ (a) and $k_D L = 4$ (b). Regions near the point $R = L$ are shown in an enlarged scale in insertions.

computational cell. Only for the computational cell of the sc lattice this may be achieved by placing macroparticles at the points with coordinates $x_i = ia$, $y_j = ja$, $z_k = ka$ if $k = 2\ell$ and $z_k = (k - 1)a + R$ if $k = 2\ell + 1$. Here i, j, k , and ℓ are the integers $(0, \pm 1, \pm 2, \dots)$. To determine the force acting on any macroparticle in the ensemble of macroparticles interacting by the Debye potential we have:

$$F_{\Sigma} = -e^2 q^2 \frac{\partial}{\partial R} \left(\sum_i \sum_j \sum_k \frac{1}{r_{ijk}} e^{-k_D r_{ijk}} \right), \quad (20)$$

where

$$r_{ijk} = \sqrt{x_i^2 + y_j^2 + z_k^2}.$$

Symbols in figure 4 present the dependencies of the interaction forces on the interparticle distance, which were calculated from (20) (the data for $k_D L = 3$ and $k_D L = 4$ are not shown to order of avoid overloading the figure). We see a good agreement of these results with the data obtained on the basis of numerical solution of equation (17). Thus we can conclude that the interaction of any pair of macroparticles is described by the Debye potential and the total force acting on any chosen macroparticle is determined by the spatial distribution of macroparticles.

The good agreement of the results obtained by the numerical solution of system (17) with the data calculated from (20) also leads to the conclusion that the method proposed in the present paper for solving the boundary value problems is fairly accurate and can be used for the solution of similar problems having a complex shape of the outer boundary.

4. Conclusion

In the present paper, the interaction of two charged pointlike macroparticles embedded in the finite size cells in an equilibrium plasma is studied. The calculations show that the shape of the outer boundary has a strong influence on the electrostatic interaction of two macroparticles and the interaction force switches from repulsion at small interparticle distances to attraction as the interparticle distance approaches the half-length of the computational cell. It is found that in the case of the computational cell corresponding to two adjacent WS cells of the simple cubic

lattice the electrostatic force acting on any macroparticle is determined by the Debye interaction of this macroparticle with all the other macroparticles. This allows us to conclude that the pair interaction potential of macroparticles in an equilibrium plasma is the Debye potential.

Acknowledgments

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References

- [1] Gundienkov V A and Yakovlenko S I 2002 *J. Exp. Theor. Phys.* **95** 864–877
- [2] Markes M E and Williams P F 2000 *Phys. Lett. A* **278** 152–158
- [3] Ignatov A M 2001 *Phys.-Usp.* **44** 199–202
- [4] Filippov A V, Pal' A F, Starostin A N and Ivanov A S 2006 *JETP Lett.* **83** 546–552
- [5] Itou H, Amano T and Hoshino M 2014 *Phys. Plasmas* **21** 123707
- [6] Lampe M and Joyce G 2015 *Phys. Plasmas* **22** 023704
- [7] Filippov A V, Pal A F and Starostin A N 2015 *J. Exp. Theor. Phys.* **121** 909–923
- [8] Neu J C 1999 *Phys. Rev. Lett.* **82** 1072–1074
- [9] Sader J E and Chan D Y C 1999 *J. Colloid Interface Sci.* **213** 268–269
- [10] Sader J E and Chan D Y C 2000 *Langmuir* **16** 324–331
- [11] Filippov A V 2016 *Contr. Plasma Phys.* **56** 1–11
- [12] Debye P and Hückel E 1923 *Phys. Zeitschr.* **24** 185–206
- [13] Ziman J M 1972 *Principles of the Theory of Solids* 2nd ed (Cambridge: Cambridge University Press)
- [14] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (New York: Holt, Rinehart and Winston)
- [15] Carslaw H S and Jaeger J C 1959 *Conduction of Heat in Solids* 2nd ed (Oxford: Clarendon)
- [16] Watson G N 1922 *A Treatise on the Theory of Bessel Functions* (London: Cambridge University Press)
- [17] Filippov A V 2009 *J. Exp. Theor. Phys.* **109** 516–529
- [18] Filippov A V 2009 *Contr. Plasma Phys.* **49** 431–445
- [19] Munirov V R and Filippov A V 2012 *J. Exp. Theor. Phys.* **115** 527–534
- [20] Munirov V R and Filippov A V 2013 *J. Exp. Theor. Phys.* **117** 809–819