Macroions non-linear screening in complex plasma

I A Martynova\textsuperscript{1,2}, I L Iosilevskiy\textsuperscript{1,2} and A A Shagayda\textsuperscript{3}

\textsuperscript{1} Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13
Bldg 2, Moscow 125412, Russia
\textsuperscript{2} Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141700, Russia
\textsuperscript{3} The State Scientific Centre of the Russian Federation Federal State Unitary Enterprise
Keldysh Research Center, Onezhskaya 8, Moscow 125438, Russia

E-mail: martina1204@yandex.ru

Abstract. The base for consideration is the well-known phase diagram of dusty plasma for an equilibrium charged system with the Yukawa potential in $\Gamma$–$\kappa$ plane, where $\Gamma$ is a Coulomb non-ideality parameter, $\kappa$ is a screening parameter, from [Hamaguchi S et al 1997 Phys. Rev. E 92 4671]. Two-component highly asymmetric electroneutral systems of classical macroions with the charge $Z$ and point-like opposite charged microions are considered in the case of big non-uniformity around macroions. Linear screening approximation is not valid for a considerable part of characteristic parameters of substantial dusty plasma. The Poisson–Boltzmann equation is solved numerically in electroneutral Wigner–Seitz cell to consider non-linear screening of a macroion by microions. Distributions of microions and non-linear potentials are calculated. This allows to make charge renormalization and to consider not a real charge $Z$ but an effective one $Z^\ast$. Also, it is shown that the initial phase changes as non-linear screening is taken into account.

1. Introduction

Phase transitions in complex plasmas have attracted interest for many years. Some of systems which are usually intended by “complex plasma” are dusty plasma of gas discharges, CDP plasma (plasma with condensed dispersed phase), colloidal plasma and dusty plasma in noctilucent clouds. In the present paper we consider equilibrium systems which consists of macroions with charge number $Z$ ($Z \gg 1$), concentration $n_Z$, temperature $T_Z$ and radius $R_Z$ and point-like opposite charged microions with charge number $1$, density $n_i$ and temperature $T_i$. Sorts of microions can be one or two ($+1$ and $−1$, for example) like in dusty plasma of gas discharges but in the present paper we consider only two-component models (macroions and one sort of microions).

All of the mentioned systems are often characterized by two dimensionless parameters:

$$
\Gamma = \frac{(Ze)^2}{kT_Z} \left(\frac{4\pi n_Z}{3}\right)^{1/3}, \quad \kappa = \frac{a}{r_D},
$$

where $a = (3/(4\pi n_Z))^{1/3}$ and $r_D = [kT_i/(4\pi e^2\langle n_i \rangle)]^{1/2}$ are the radii of Wigner–Seitz and Debye, respectively; $\langle n_i \rangle$ is the microions averaged concentration in a considered volume ($\langle n_i \rangle = Zn_Z$).

Representative quantities of the mentioned systems are the following: $\Gamma \sim 10^2–10^5$, $\kappa \sim 0–10$, $Z \sim 10^3–10^4$, $n_Z \sim 10^3–10^4 \text{ cm}^{-3}$, $T_Z \sim 1–2$ eV, $T_i \approx 0.03$ eV (temperature of positive...
microions) and \( T_e \sim 1–7 \) eV (temperature of electrons) for dusty plasma of gas discharges [1]; \( \Gamma \sim 10–10^5, \kappa \sim 0–10, Z \sim 10–10^5, n_Z \sim 10^8–10^{14} \) cm\(^{-3}\), \( T_i \sim 2000–3000 \) K for CDP plasma [2]; \( \Gamma \sim 10–10^3, \kappa \sim 0–10, Z \sim 10–10^3 \) for colloidal plasma (see [3], for example); \( \Gamma \sim 1, \kappa \sim 0–10, Z \sim 10^2, T_Z = T_i = T_e \approx 0.03 \) eV for dusty plasma in noctilucent clouds [4]. Temperatures of macro- and microions can be considered as equal for CDP and colloidal plasmas.

Screening of complex plasmas charges is one of the basic properties which has been discussed for many years. At first, the linear Debye–Hückel (DH) approximation was used to get the potential of the Yukawa form:

\[
\varphi_{Yu}(r) = \frac{Ze}{r} \exp \left( -\frac{r}{\kappa_D} \right). \tag{2}
\]

A phase diagram of complex plasma was obtained in 1997 by methods of direct numerical simulations [5]. A potential is assumed to be of the Yukawa form. This potential was obtained from the Poisson–Boltzmann equation

\[
\Delta \varphi(r) = -4\pi\langle n_i \rangle e \exp \left( -\frac{e\varphi(r)}{kT_i} \right), \tag{3}
\]

and the linearization condition \( e\varphi(r)/(kT_i) \ll 1 \) was used. For example, the Poisson–Boltzmann equation was solved in [6], and there the linearization condition was taken into account. But this condition is not valid for all representative quantities of complex plasmas. Non-linear screening was considered by different authors in equilibrium [2, 7–9] and non-equilibrium (see, for instance, [10]) systems. It was shown in [7–9] that microions were attracted by the opposite charged macroion so that the real macroion charge (from now on we call \( Z \) not a charge number but a charge) seemed to be smaller over large distances and was called an effective one (\( Z^* \)).

Moreover, it means that we should also consider effective parameter of Coulomb non-ideality \( \Gamma^* \) and effective structural parameter \( \kappa^* \)

\[
\Gamma^* = \left( \frac{Z^* e}{kT_i} \right)^2 \left( \frac{4\pi}{3} n_Z \right)^{1/3}, \quad \kappa^* = \left( \frac{3}{4\pi n_Z} \right)^{1/3} \left( \frac{4\pi e^2 n_{i0}}{kT_i} \right)^{1/2}, \tag{4}
\]

where \( n_{i0} \) is microions concentration at infinity from a sampling macroion (or on the boundary of the spherically symmetric cell).

We made an assumption that the initial phase diagram is valid for effective \( \Gamma^* \) and \( \kappa^* \). In this paper we solve the Poisson–Boltzmann equation to find effective charges for different parameters of complex plasma. Also, we show that the phase diagram differs if one replots it from \( \kappa^*–\Gamma^* \) plane to \( \kappa–\Gamma \) one.

The paper is organized as follows. Non-linear screening is considered in section 2. Section 3 presents the ways of determination of the effective charge. Then, in section 4 we discuss how the phase diagram [5] changes its look while reploting \( \kappa^*–\Gamma^* \) plane to \( \kappa–\Gamma \) one. In section 5 we make conclusions.

### 2. Non-linear screening

We showed in figure 1 that the majority of representative quantities don’t comply with the linearization condition. Also, it is seen that concentration of a macroions subsystem is restricted above because of impossibility to compress it infinitely.

We consider spherically-symmetric electroneutral cell with a macroion with charge number \( Z \) and radius \( R_Z \) in the center of the cell. Its radius is \( R \) where \( (4/3)\pi R^3 n_Z = 1 \), \( n_Z \) is macroions concentration. There are point-like microions with charge number +1 in the cell beside a macroion. Thus, we have

\[
Z = \int_{R_Z}^{R} 4\pi r^2 n_{i0} \exp \left( -\frac{e\varphi(r)}{kT_i} \right) dr. \tag{5}
\]
Figure 1. Linear screening boundaries $kT_{\text{min}} = Z e^2 / R_Z$ (line (A) for a macroion with the radius $R_Z = 10 \, \mu m$ and line (B) for $R_Z = 1 \, \mu m$) and macroion concentration boundaries $n_{\text{max}}$ (line (C) for $R_Z = 1 \, \mu m$ and line (D) for $R_Z = 10 \, \mu m$), where $n_{\text{max}} R^3 = 1$ for $Z = 100$ (a) and $Z = 300$ (b). Yellow, pink and blue rectangles are areas of representative quantities of dusty plasma of gas discharges, CDP plasma and dusty plasma in noctilucent clouds respectively.
By Gauss’s law
\[ r^2 E(r) = q(r), \]  
where \( q(r) \) is a total charge in the sphere with the radius \( r \), \( E(r) \) is total intensity of the electrical field. So,
\[ E(r) = \frac{e}{r^2} \left( Z - \int_{R_z}^r 4\pi r_1^2 n_0 \exp \left( -\frac{e\varphi(r_1)}{kT_1} \right) d\varphi_1 \right). \]  
Using (5) and (7) we have
\[ E(r) = \frac{Ze}{r^2} \left( 1 - \int_{R_z}^r 4\pi r_1^2 \exp \left( -\frac{e\varphi(r_1)}{kT_1} \right) d\varphi_1 \right). \]  
Then we consider reduced variables: \( \Phi(r) = \frac{e}{kT_i}\varphi(r), x = (1/R)r, E = [eR/(kT_i)]E \) and have
\[ E(x) = \frac{\delta^2}{3} \frac{1}{x^2} \left( 1 - \int_{x_Z}^x 4\pi x_1^2 \exp(-\Phi(x_1)) dx_1 \right), \]  
where \( x_Z = R_z/R \) and
\[ \delta^2 = \frac{3Ze^2}{kT_i R}. \]  
What is the physical sense of the parameter \( \delta^2 \)? Cell averaged macroion concentration can be written as
\[ \langle n_Z \rangle = \frac{3Z}{4\pi R^3}. \]  
Then we have
\[ \langle r_D \rangle^2 = \frac{kT_1}{e\langle n_Z \rangle} = \frac{4\pi kT_1}{3Ze} R^3 \]  
and
\[ \delta^2 = \frac{R^2}{\langle r_D \rangle^2}. \]  
So,
\[ E(x) = \frac{3Ze^2}{3kT_i R x^2} \left( 1 - \int_{x_Z}^x 4\pi x_1^2 \exp(-\Phi(x_1)) dx_1 \right), \]  
and
\[ \frac{d\Phi}{dx} = -E(x), \]  
where \( x \in [0, 1] \). The boundary condition is \( \Phi(1) = 0 \) (\( E(1) = 0 \) is valid by itself).

We compared our results with [7]. Thus, we present some new parameters
\[ \chi = \frac{Ze^2}{kT_i R Z}, \]  
and
\[ \Gamma_{ii} = \frac{e^2}{kT_i} (4\pi n_i)^{1/3}. \]
Figure 2. Self-consistent potentials as solutions of the Poisson–Boltzmann equation. Black line is based on [7], red points are obtained by us (Z = 25, \( \chi = 45, \Gamma_{ii} = 0.1 \)).

The results of our comparison are shown on figure 2. Our solution practically coincides with the one from [7]. The Poisson–Boltzmann equation was solved analytically in [9], and this solution also coincides with one from [7].

Moreover, we compared potential which is the solution of (14) and (15), Debye–Hückel potential and one which corresponds to a cell with a macroion and microions whose profile is uniform (figure 3). The second potential was obtained from

\[
\varphi_{LDH} = \begin{cases} 
C_1 \exp(\kappa_{LDH} r) + C_2 \exp(-\kappa_{LDH} r) + \varphi_1 & \text{for } R_Z \leq r \leq R, \\
0 & \text{for } r \geq R.
\end{cases} 
\]  

(18)

Then we solved the Poisson–Boltzmann equation using the linearization condition

\[
\Delta \varphi_{LDH}(r) = -4\pi e n_{LDH0} \left( 1 + \frac{e \varphi_{LDH}(r)}{k T_i} \right)
\]

(19)

and set equal two macroion border potentials, then two cell border potentials, next two macroion border potential gradients and, finally, two cell border potential gradients. We had

\[
\Phi_{LDH}(r) = -\frac{R \exp(\kappa_{LDH} R)}{\exp(\kappa_{LDH}(R + 1)) + \exp(\kappa_{LDH} R - 1)} + 1,
\]

(20)

where \( \Phi_{LDH}(r) = e \varphi_{LDH}(r)/(k T_i) \).

We also obtained a potential in the case when microions have uniform profile (\( n_{UPi} = \text{const} \)):

\[
\varphi_{UP} = \begin{cases} 
C_3 r^2 + \frac{C_4}{r} + \varphi_2 & \text{for } R_Z \leq r \leq R, \\
0 & \text{for } r \geq R.
\end{cases} 
\]  

(21)

Thus,

\[
\Phi_{UP} = \frac{e \varphi_{UP}(r)}{k T_i} = \frac{Ze^2}{k T_i} - 0.5 \frac{R^3 - R_2^3}{R^3 - R_Z^3} \frac{1}{R^3 - R_Z^3} - \frac{1.5}{R^3 - R_Z^3} R^3 - R_2^3 R^2. 
\]  

(22)
Figure 3. Self-consistent potentials: (a) \( n_Z = 10^8 \text{ cm}^{-3}, R = 13.4 \mu \text{m}, R_Z = 1.34 \mu \text{m}; \) (b) \( n_Z = 10^6 \text{ cm}^{-3}, R = 62 \mu \text{m}, R_Z = 6.2 \mu \text{m}; \) (A)—the solution of the Poisson–Boltzmann (PB) equation; (B)—the solution of the Poisson–Boltzmann equation using the linear condition; (C)—potential as microions have uniform profile; \( Z = 1000, kT_i = 0.03 \text{ eV} \) is microions temperature.

Microions distribution which is obtained using the Poisson–Boltzmann equation is

\[
n_i(r) = n_{i0} \exp \Phi(r).
\]

Microions distribution based on solution the Poisson–Boltzmann equation using the linearization condition is

\[
n_{LDHi}(r) = n_{LDHi0}(1 + \Phi_{LDH}(r)).
\]

There are microions distributions in figure 4.

It is well known that the Poisson–Boltzmann equation doesn’t take into account microions size and their correlations. Thus, we obtained parameters of Coulomb non-ideality \( \Gamma_{ii} \) for the mentioned before quantities. It is obvious that maximum value of \( \Gamma_{ii} \) is \( \Gamma_{iimax} = \Gamma_i(R_Z) \). The maximum microions concentration we have obtained gave the maximum \( \Gamma_{iimax} \approx 0.547 \) (figure 5). This figure indicates that \( \Gamma_{ii} < 1 \) (mainly, \( \Gamma_{ii} \ll 1 \)) and we can neglect microions correlations for these quantities and use the Poisson–Boltzmann equation.

3. Effective charge

We compared dependences \( q(r) \) which were obtained by [7] and us (see figure 2). The difference between the lines at large distances can be explained easily. Bystrenko and Zagorodny considered not a two-component model but a three-component one (with two sorts of microions with the charges +1 and −1). Moreover, they considered a sample microion in infinite electroneutral background plasma, and we solved the Poisson–Boltzmann equation in an electroneutral cell which consists of a macroions and opposite charged microions.

Moreover, we compared three ways to determine an effective charge. The first way is well-known and based on the following idea. All microions with concentration which is the same as on the border of the cell are named as free. Total value of unbound microions is the same as the value of the effective charge. The rest microions are considered as bound (see [11] for details, for instance). We suggested two more ways of the effective charge determination. The second way follows from figure 6 itself. It is logical to assume that value of effective charge can be found right at the point of maximum curvature \( r_{infl} \) of the curve. It means that microions at
Figure 4. Microions distributions: (a) \( n_Z = 10^8 \text{ cm}^{-3}, R = 13.4 \text{ \mu m}, R_Z = 1.34 \text{ \mu m} \); (b) \( n_Z = 10^6 \text{ cm}^{-3} \); (A)—the solution of the Poisson–Boltzmann equation; (B)—the solution of the Poisson–Boltzmann equation using the linear condition; (C)—the microions uniform profile; \( Z = 1000, kT_i = 0.03 \text{ eV} \).

Figure 5. Parameter of Coulomb non-ideality (microion–microion): \( Z = 1000, n_Z = 10^8 \text{ cm}^{-3}, R = 13.4 \text{ \mu m}, R_Z = 1.34 \text{ \mu m}, kT_i = 0.03 \text{ eV} \).

\( r < r_{\text{infl}} \) are bound, and the rest are free. And, finally, the third way is based on the invalidity of the linearization condition \( e\varphi(r)/(kT_i) \ll 1 \). Let us assume that \( e\varphi(r_{\text{inv}})/(kT_i) = 1 \). Thus, we suggest to consider all microions at \( r < r_{\text{inv}} \) as bound. The others microions can be named as free. We illustrate the ways to determine an effective charge in figures 6 and 7.
Figure 6. Total charge $q$ in the sphere of radius $r$. Line (A) is based on [11]. Line (B) is based on our calculations. $Z = 25$, $\chi = 20$, $\Gamma = 0.1$. Two ways to determine the effective charge are illustrated. Right black point is the effective charge which is determined as a charge at the maximum curvature point. Left black point is the effective charge which is determined like in [11] (through cell border concentration).

Figure 7. Total charge $q$ in the sphere of radius $r$: $Z = 1000$, $n_Z = 10^8$ cm$^{-3}$, $R = 13.4$ µm, $R_Z = 1.34$ µm, $kT_i = 0.03$ eV. Left red point is the effective charge at the point at which $e\varphi(r)/(kT_i) = 1$. Right red point is the effective charge which is determined like in [11] (through cell border concentration).
Figure 8. Phase diagram of dusty plasma [7] and points that illustrate how phase state differs as non-linear screening is taken into account. Points 1, 2, 3, 4 correspond to \((\kappa, \Gamma)\), triangles \(1^*, 2^*, 3^*, 4^*\) correspond to \((\kappa^*, \Gamma^*)\) (calculation based on the way of determination the effective charge in cell border concentration). \(Z = 1000, kT_i = 0.03\) eV. Point 1: \(n_Z = 10^8\) cm\(^{-3}\). Point 2: \(n_Z = 10^7\) cm\(^{-3}\). Point 3: \(n_Z = 10^6\) cm\(^{-3}\). Point 4: \(n_Z = 10^5\) cm\(^{-3}\).

4. The phase diagram of dusty plasma and non-linear screening

So, as non-linear screening is taken into account all phase states move in \(\kappa - \Gamma\) plane (figure 8). For example, if one thinks that they consider fcc lattice (point 1) it is not valid. The real state for point 1 is fluid as non-linear screening is taken into account.

5. Conclusions

We solved the Poisson–Boltzmann equation in the electroneutral cell with a macroion in the center. Our aim was to consider non-linear screening and to obtain effective charges for different quantities. We calculated effective charges \(Z^*\) by three methods. The first one is quite common. All microions with the same density like on the cell border are considered as free, and their total charge is the effective one. We suggest two more ways of the effective charge determination. The second way is based on the look of the dependence \(q(r)\) (total charge in the sphere with radius \(r\)). This dependence has maximum curvature, and sometimes it is strongly pronounced like in figure 6. However, it is hard to determine the point of maximum curvature \(r_{\text{infl}}\) for some cases. Anyway, we think it is fair to consider all microions that are situated to a macroion closer than the border of the sphere with the radius \(r_{\text{infl}}\) as bound. Finally, the third way is based on invalidity of the linearization condition. Thus, microions which are situated closer than the radius of the sphere \(r_{\text{inv}}\) are bound, where \(e\varphi(r_{\text{inv}})/(kT_i) = 1\). Also, we proved that we can neglect microion-microion correlations as the corresponding parameter of Coulomb non-ideality \(\Gamma_{ii} \ll 1\).

Moreover, we made an assumption that a real phase state [5] is determined by effective values \(\Gamma^*\) and \(\kappa^*\). Taking into account non-linear screening leads to a situation when a phase state for \((\kappa, \Gamma)\) is different as for the corresponding point \((\kappa^*, \Gamma^*)\). Thus, we showed how the phase state [5] changes from \((\kappa^*, \Gamma^*)\) plane to \((\kappa, \Gamma)\) one.
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