CRITICAL EFFECTS IN SCREENING OF FINITE-SIZE CHARGES IN PLASMAS

O. Bystrenko and A. Zagorodny

Bogolyubov Institute for Theoretical Physics, 252143, Kiev, Ukraine

Colloidal plasmas, such as dusty plasmas and charged colloidal suspensions, attracted considerable attention in recent years as physical systems, where interesting space ordering phenomena may be observed [1-2]. Typically, colloidal plasmas consist of a large number of highly charged ($Z \simeq 10^3 - 10^6$) colloidal particles (grains) immersed in a weakly coupled plasma background. Due to strong Coulomb repulsion between grains the colloidal component may exhibit a correlated behavior and even form a crystalline (Coulomb) lattice. The simplest and fundamental questions concerning such systems should be those of the effective screened field around a single high-Z grain and of the effective interactions between grains. To make estimates of physical properties, and even to perform Monte-Carlo (MC) or molecular dynamics computer simulations [3], one frequently uses as effective interactions the Yukawa-like potentials resulting from the linear Debye-Hückel (DH) screening theory. However, its validity in the case of a high-Z impurity in a plasma background is *a priori* unclear, what can be shown as follows. The DH screening theory can be obtained as a linear approximation within the Poisson-Boltzmann (PB) approach based on the equation

$$\Delta\varphi(r) = -4\pi Ze\delta(r) - 4\pi en\{exp[-\frac{e\varphi(r)}{kT}] - exp[\frac{e\varphi(r)}{kT}]\} \tag{1}$$

describing plasma as a two-component gas with Boltzmann distribution. Here φ is the screened self-consistent potential; e - the charge of a positively charged plasma particle; n - plasma concentration at infinity; k - Boltzmann's constant; T - temperature.

For a spherical particle (grain) of a radius a, the assumption $e\varphi/kT \ll 1$ yields, after linearization with respect to φ, the well-known solution in the form

$$\varphi(r) = \frac{Z'e}{r}exp(-\frac{r}{r_D}) \tag{2}$$

with the effective charge $Z' = Zexp(\sigma)/(1+\sigma)$, where $\sigma = a/r_D$, and r_D denotes the Debye screening length. However, at short distances the above assumption is for sure violated, what makes the transition $a \to 0$ with the DH limit

$$\varphi_D(r) = \frac{Ze}{r}exp(-\frac{r}{r_D}) \tag{3}$$

incorrect. In actual fact in the case of a grain of a small size nonlinear effects in screening might be of importance and direct applicability of Eq.(2) would break down. To estimate the validity of the linear approximation, it is convenient to introduce the quantity

$$\chi = \frac{Ze^2}{kTa}$$

representing the ratio of potential energy of a plasma particle to the kinetic one on the surface of the charged grain. Dusty plasmas with high Z impurities and charged colloidal suspensions provide examples of physical systems with χ on the order of $1-10$, what casts doubt on the validity of the linear DH theory for the description of screening.

It should be noted that the effects of nonlinear screening in the context of colloidal suspensions were considered in Ref.[4], and the results of that work correlate qualitatively with ours. Nevertheless, microscopic MC simulations on the above problem are of especial importance. The point is that the PB approach is based on the concept of effective field, which requires that the plasma-plasma must be negligibly small. As will be seen from the results obtained, the nonlinear screening effects in a sharp 'plasma condensation' near the grain surface, what casts doubts on the validity of the mean field approximation.

In the present work we consider the problem of screening of a finite-size charge $Z \gg 1$ in a plasma background (for the case of $\chi \simeq 1-50$) in two ways: by using the method of MC simulations and via correct account of nonlinear effects within the PB approach.

Let us say a few words about the choice of parameters. The PB theory is based on the notion of the effective mean field, which loses its meaning for strongly coupled ($\Gamma = e^2/kTd \geq 1$, where $d = (4\pi n)^{-1/3}$) plasmas,as the plasma correlations become significant. Typical for colloidal plasmas are the values $Z \gg 1$, $\Gamma \ll 1$. We present below mainly the results for $Z = 25$, $\Gamma = 0.1$, $\chi = 2, 10, 20, 40$.

The MC simulations of screening were performed in the model, in which the two-component plasma background was represented by sufficiently large number ($N = 375$) of charged hard spheres confined in a spherical volume with a grain of $Z = 25$ fixed in the centre. The charge of a plasma particle and plasma temperature corresponded to the coupling constant $\Gamma = 0.1$ providing the Debye screening length $r_D = 0.28$ of the radius of the spherical volume. The volume fraction of plasma component was $v_p = 5 \cdot 10^{-6}$, small enough to reduce the plasma hard core correlations, but sufficiently large to prevent collapsing (sticking together) plasma particles. The radius of the central charged grain was set subsequently equal to $a/r_D = 0.61, 0.11, 0.047, 0.017$, which was defined by the given values $\chi = 2, 10, 20, 40$.

Simulations were carried out for NVT-ensemble using the conventional Metropolis algorithm. After relaxation, every 375th of the next 3,750,000 configurations was included into the ensemble, so that the total averaging was performed over 10,000 statistically independent configurations.

To take into account nonlinear effects within the PB approach, we solved the Eq.(1) numerically, by using the shooting techniques and the second-order Runge-Cutta numerical algorithm . The boundary conditions we used defined the electric field on the surface of the grain and the potential at infinity. The number of points dividing the domain of solution was $N = 10^4$- 10^6. The accuracy of computations was checked to be within the range of 10^{-5}.

In numerical computations there were investigated:

1) effective (screened) potential $\varphi(r)$ and the ratio $\varphi(r)/\varphi_D(r)$, - in order to find out the influence of nonlinear effects and to check the asymptotical behavior of $\varphi(r)$ and to find the (relative) effective charge Z^* from the relation $Z^* = \varphi/\varphi_D$ at $r \gg r_D$;

2) charge distribution function $Q(r)$ defined as a total relative charge residing within a sphere of a radius r;

Our computations have shown a good agreement between microscopic MC results and the nonlinear PB approach. A distinct difference between the present results and the linear DH theory was detected at large χ, as nonlinear effects became more significant (Figs. 1-3). In this case the effective charge tends to diminish with growing χ, so that $Z^* \to 0$ with $\chi \to \infty$, or, respectively, with $a/r_D \to 0$.The screened potential in the vicinity of the grain surface loses its Yukawa-like form given by the Eq.(2). The character of charge distributions (Figs. 4) indicates that the decrease in effective charge for large χ is accompanied by accumulation of corresponding portions of induced charge on the surface of charged sphere; the rest of it is distributed around and produces at distances the usual Debye-like screening. The point of the beginning of that 'condensation' in all the cases (i.e. for all sets of parameters Z and Γ, etc. in our computations) was estimated as $\chi = 4 - 5$.

It is interesting to note that MC simulations of infinite asymmetric two-component (colloidal) plasmas performed in Ref.[5] indicated at $\chi > 6$ a sort of peculiar condensation of plasma particles on the surface of grains. In that work this phenomenon was connected with a phase transition, specifically, in view of an express increase in heat capacity and appearance of short-range plasma-plasma correlations in this region. Apparent similarity of the results suggests that we deal with the same phenomenon, which means, in its turn that the description of a phase transition is possible within the PB theory based on the concept of a gas in a self-consistent field. This rather unexpected conclusion may be more explainable, if we recall that the given value Z defining the ratio of the charge of the grain to that of a plasma particle, introduces a microscopicity into the model and may provide a possibility of critical phenomena.

Acknowledgements

In conclusion, we would like to thank Prof. P. Schram for valuable discussions. This work was supported in part by the State Fund of Fundamental Research of Ukraine (grant No. 2.4/319) and by the International Association INTAS (project No. 96-0617).

References

[1] H. Thomas et al: Phys. Rev. Lett. **73**, 652 (1994)

[2] P. Pieransky: Contemp. Phys. **24**, 25 (1983)

[3] M.O. Robbins, K. Kremer and G.S. Grest: J. Chem. Phys. **88**, 3286 (1988)

[4] S. Alexander et al: J. Chem. Phys. **80**, 5776 (1984)

[5] O. Bystrenko and A. Zagorodny: Europhys. Conf. Abstr. **21A**, 1385 (1997)

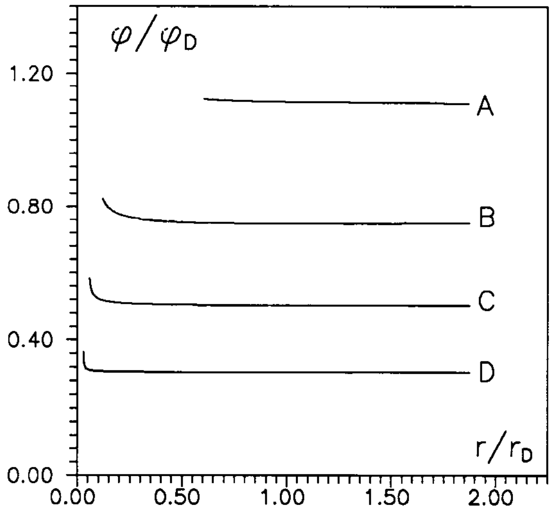

Figure 1. Ratio φ/φ_D of effective potentials (φ - the nonlinear PB approach, φ_D - DH approximation vs. distance for χ=2(A), 10(B), 20(C), 40(D). Constant values of the ratios at distances evidence the Yukawa-like asymptotical behavior of screened potential.

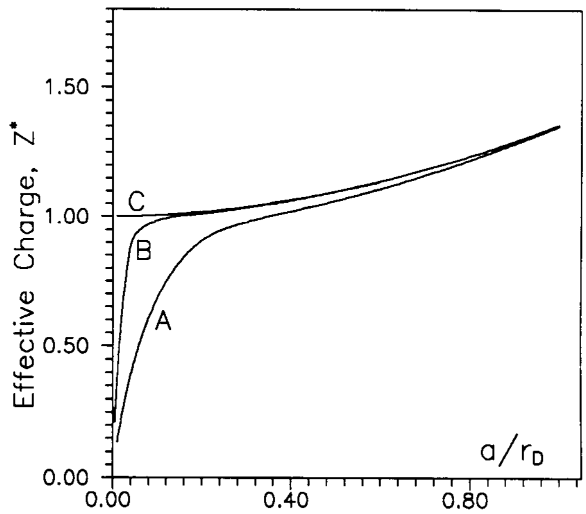

Figure 2. Effective charge Z^* vs. diameter of the grain, defined as $Z^* = \varphi/\varphi_D$ at large r. $Z = 25,\ \Gamma = 0.1$(A); 0.05(B). The line (C) corresponds to the linear DH approximation. Account of nonlinearity gives rise to a sharp decrease in effective charge at small radii a.

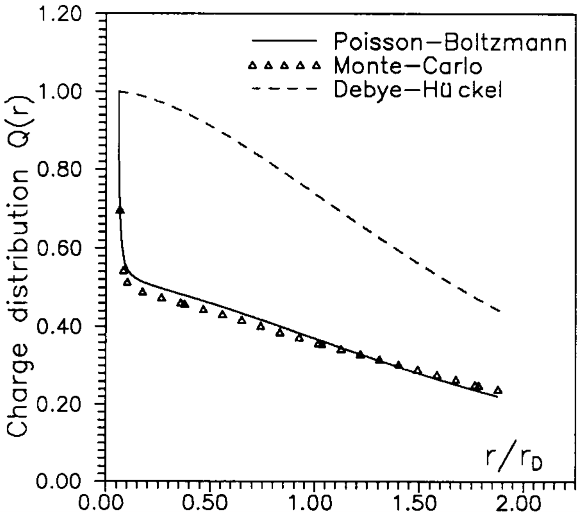

Figure 3. Charge distributions $Q(r)$ near the charged grain for $Z = 25, \Gamma = 0.1, \chi = 20$. Dashed line - linear DH theory; solid line - nonlinear PB approach; symbols - results of MC simulations. A sharp step-wise change in distribution means an accumulation of plasma charge on the grain surface.

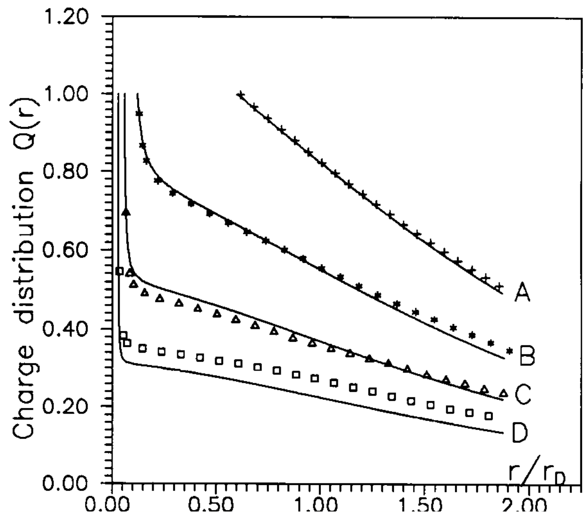

Figure 4. Charge distributions of $Q(r)$ near the charged grain for $Z = 25, \Gamma = 0.1$. Solid lines - nonlinear theory; sumbols - results of MC simulations. χ=2(A), 10(B), 20(C), 40(D).