Nonlinear Poisson-Boltzmann equation in spherical symmetry

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The Poisson-Boltzmann problem in spherical symmetry has been considered using the distribution of a self-consistent potential around a charged grain in a thermal collisional plasma as an example. The qualitative patterns of all possible solutions have been presented and a study of their asymptotics has been carried out. It has been demonstrated that for large potentials it is possible to neglect the curvature of the grain surface and to use the solution of the plane problem. It has also been demonstrated that the electrical interaction of the grains is possible only at distances smaller than eight screening lengths.

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I. INTRODUCTION

The Poisson equation

$$\Delta\varphi = -4\pi\rho \tag{1}$$

is applicable to the description of the spatial distribution of the electrostatic potential φ in a system with volume charge density ρ. This problem often arises in research into colloid suspensions and dusty plasma. Both these systems contain free charged particles of the medium (ions and electrons) and larger formations [colloidal particles (macroions) in colloid suspensions and dust grains in a dusty plasma], which also get a charge. In both cases, the charged grains (or macroions) form a space-charge region that screens the charge of the grain. The charged grain is the source of an electric field that separates the electrons and ions near the grain surface, and provides for the emergence of a volumetric charge. On the other hand, the volumetric charge near the grain surface influences the spatial distribution of the potential and the field. Thus, there is a self-consistent problem in defining the spatial distribution of the electric field and the number densities of the charge carriers.

For the solution of this problem it is convenient to present the number density of charge carriers in the form of the Boltzmann factor $n \sim \exp(-q\varphi/T)$, where q is the charge. In this case there is a self-consistent Poisson-Boltzmann equation

$$\Delta\varphi = -4\pi\sum_j q_j n_{j0} \exp\frac{-q_j\varphi}{T}, \tag{2}$$

which is the nonlinear differential equation for the potential φ.

This representation is quite suitable for colloid suspensions [1–4], but for dusty plasmas special substantiation is necessary. For example, a gas-discharge collisionless dusty plasma is not an equilibrium system; therefore the Boltzmann factor is not applicable to it [5], except for those cases when $e\varphi \ll T$ [6] and the Boltzmann factor is used in the linearized form [7,8]. Otherwise it is necessary to use other approaches that are based on the motion of particles [8–10].

However, in a thermal collisional plasma there is a local thermodynamic equilibrium that makes it possible to use the Boltzmann factor [11–15]. A laboratory thermal dusty plasma [16] (or smoky plasma) is an isothermal system and represents a gas at atmospheric or higher pressure and at the temperatures of 1500–3500 K. Ionization in a thermal plasma occurs due to collisions between gas particles; therefore such a plasma is strongly collisional, unlike the low-pressure gas-discharge plasma. It usually contains easily ionizable atoms of alkali metals, as natural impurities or in the form of special additional agents, which are the basic suppliers of free electrons and singly charged positive ions. A smoky plasma is formed in the area of condensation of the products of combustion of a hydrocarbon or metallized fuels.

Thus, the potential distribution around a single grain in a collision thermal plasma, as well as in colloid systems, is described by the spherically symmetrical Poisson-Boltzmann equation, which can be presented in the following form:

$$\frac{d^2\varphi}{dr^2} + \frac{2}{r}\frac{d\varphi}{dr} = 4\pi e\left(n_e^* \exp\frac{e\varphi}{T} - n_i^* \exp\frac{-e\varphi}{T}\right), \tag{3}$$

where n_e^* and n_i^* are the electron and ion number densities at some point r^*, where the potential is equal to zero. It should be noted that the zero value of the potential at some point does not at all mean a lack of field; therefore we cannot *a priori* approve the equality of the number densities n_e^* and n_i^*.

A common solution of Eq. (3) is not known, therefore various approaches are used. So, for example, in Ref. [11], for particles with large radius it is suggested to neglect the term $(2/r)\varphi'$, and for particles with small radius to use the approach $\Delta\varphi \sim 0$, i.e., the Coulomb potential. However, in Ref. [17], it is shown that the Coulomb-type potential is not applicable, because the image charge effect is essential near the grain surface and a modification of the Debye potential is made due to nonlinear corrections in the Boltzmann distribution.

The Debye potential is the solution of the linearized Eq. (3). Linearization is possible for small potentials; however, we were recently surprised to find that the Debye distribution is used for large potentials, when linearization of the Poisson equation is impossible. Therefore, we consider it necessary to carry out a detailed analysis of the Poisson-Boltzmann equation.

The studies of the Poisson-Boltzmann equations made by other authors earlier are based on approaches that consider the physical features of the system. In the present paper, a detailed mathematical analysis of the spherically symmetrical Poisson-Boltzmann equation, irrespective of the field of application, has been carried out. Therefore, we, though speaking about the dust grains in a plasma for definiteness, will not consider the ranges of validity of the Poisson-Boltzmann theory as it is often used not only in plasma physics, but also in many other fields of physics.

The Poisson-Boltzmann equation is solved mostly numerically; therefore the analysis offered by us will be a good addition to the numerical solutions as it allows defining the pattern of solution in advance.

II. PRELIMINARY EXAMINATION OF THE POISSON EQUATION

We shall consider a separate grain in some volume of plasma, consisting of the electrons and single-charged ions. The number density of the grains is much less than the number density of the atoms of the added agent, which allows consideration of a separate grain in the plasma. This approach corresponds to the model of Wigner-Seitz cells, for the first time applied by Gibson [18], and in the isothermal equilibrium plasma described by Eq. (3).

For further consideration it is necessary to choose some reference point for the potential and, accordingly, for the number densities of the charge carriers. The most common, but not therefore the most correct, is a simple statement that at $r\to\infty$ $\varphi=0$. It is valid only for a single grain in an infinite plasma. If the volume of plasma is limited, at the boundary of the volume there is a space-charge layer, caused by the different mobilities of electrons and ions.

We shall use the bulk plasma potential concept that performed well both in a dust-electron plasma [19] and in a complex plasma [20]. This model assumes that the potential is calculated from some base level φ_{pl}, which depends on the charge of the gas phase. Thus, the interaction of dust grains with the plasma or the presence of an active boundary of the plasma volume leads to a change of φ_{pl}. It allows use of a single-particle approach for any grain with the boundary conditions $r\to\infty$, $\varphi=\varphi_{pl}$ or the Wigner-Seitz approach with the requirement that $\varphi\sim\varphi_{pl}$ on the boundary of the cell.

In our case, the bulk plasma potential is the trivial solution of Eq. (3)

$$\Delta\varphi_{pl}=0, \quad \varphi_{pl}=\frac{T}{2e}\ln\frac{n_i^*}{n_e^*}, \tag{4}$$

and either of the two replacements $\varphi(r)=\varphi_{pl}\pm\phi(r)$ reduces Eq. (3) to the following form:

$$\Delta\phi(r)=8\pi e\sqrt{n_e^* n_i^*}\sinh\frac{e\phi(r)}{T}. \tag{5}$$

Therefore, all the solutions of Eq. (3) are symmetrical about the line Eq. (4), and any solution that differs from the trivial solution cannot touch this trivial solution by virtue of the theorem of existence and uniqueness.

Further, we shall pay attention to the fact that, owing to oddness of the function $\sinh(x)$, the solutions having a local minimum are located in the half plane $\varphi>\varphi_{pl}$, and the solutions having a local maximum in the half plane $\varphi<\varphi_{pl}$. The solutions having an extreme correspond to repulsion of the grains. Hence, the grains repel only when both surface potentials are greater than φ_{pl}, or both are less than φ_{pl}. If the surface potentials of the neighboring grains are located on the different legs of the line Eq. (4), the grains are attracting.

The presence of an electric field in the plasma is defined by the value $\nabla\phi$ and, as will be shown further, localized in a thin layer at the grain surface. Far from the dust grain $\phi\sim 0$ and $\nabla\phi\sim 0$. In these areas, the plasma remains locally neutral (quasineutral), that is, the electron and ion number densities are equal to some value, called the unperturbed number density $n_e(\varphi_{pl})\sim n_i(\varphi_{pl})\sim n_0$, and the value φ_{pl} characterizes the size of the operation that is necessary for the volume of plasma to gain some charge Q_{pl}. In detail, the bulk plasma potential is described in Ref. [20] and for a Wigner-Seitz cell of radius $R_W=(4\pi N_d/3)^{-1/3}$ the following expression is valid:

$$\varphi_{pl}\cong-\frac{\int_a^{R_W}(rE)^2dr}{a^2E_s}, \tag{6}$$

where E_s is the field at the surface of the grain with radius a.

Let us note that the bulk plasma potential is not only a reference mark that can be shifted in any way. The bulk plasma potential is immediately related to the thermodynamic and dielectric properties of the plasma, or any other medium to which the Poisson-Boltzmann theory is applied. For example, if the perturbation factor in the plasma is only the electric field, the bulk plasma potential defines the ionization equilibrium as the additive to the ionization potential of atoms: $I_{eff}=I+e\varphi_{pl}$. Moreover, in some cases the spatial inhomogeneity of the bulk plasma potential determines the formation of the ordered structures [21].

III. ASYMPTOTIC SOLUTIONS OF THE POISSON EQUATION

Equation (5) is easily reduced to the dimensionless form by means of the change of variables $\Phi(r)=e\phi(r)/T$, $x=r/r_D$:

$$\Phi''+\frac{2}{x}\Phi'=\sinh(\Phi), \tag{7}$$

where $r_D=\sqrt{T/8\pi e^2 n_0}$ is the screening length.

Applying the transformations $v(y)=\Phi(x)$ and $y=1/x$ to Eq. (7), for the new unknown function $v(y)$ we shall obtain an equation of the form

$$\frac{d^2v}{dy^2}=y^{-4}\sinh(v). \tag{8}$$

As $v'(y)=1/y'(v)$ and $v''(y)=-y''(v)/[y'(v)]^3$, in relation to the inverse function $y(v)$ Eq. (8) will have the following form:

$$y''=-\operatorname{sgn}(y')\sinh(v)y^{-4}|y'|^3. \tag{9}$$

This equation is a special case of the more general differential equation

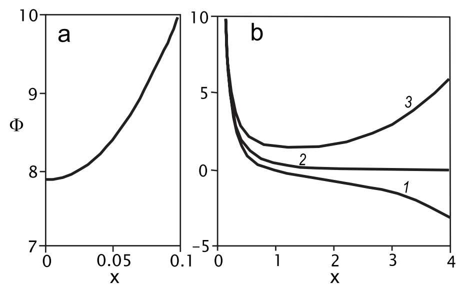

FIG. 1. Solutions of Eq. (7) for radius of grain $a=0.1r_D$. (a) Equation (11b); (b) line 2, Eq. (11c) or Eq. (11d), $\delta=0$; line 1, Eq. (11d), $\delta>0$; line 3, Eq. (11d), $\delta<0$.

$$y''=p(v)y^{\alpha}|y'|^{\beta}, \tag{10}$$

where α and β are real numbers, and p is a function continuous in some interval of the real axis.

The asymptotic formulas of all solutions of Eq. (10) as $v\uparrow v_0$ (tends to any point v_0 from below) were obtained in [22,23]. The asymptotic solutions of Eq. (10) as $v\downarrow v_0$ (tends to any point v_0 from above) can be easily obtained from those results by means of some simple replacements of an independent variable. Thus, the asymptotics of each solution of Eq. (10) can be written at any point from the closure of the range of definitions of this solution, which allows us to feature a global pattern of behavior of all solutions of Eq. (10).

By means of applying the results of Refs. [22,23] to Eq. (9), it is possible to construct a qualitative pattern of behavior of all solutions of Eq. (7), presented in Figs. 1 and 2.

We want to note the likeness of the plots Figs. 1(b) and 2(b) with the investigation made by Deryagin for the planes in an electrolyte [24]. Similar results have been obtained in Ref. [20] for inter-reacting planes in a thermal plasma. But in this case the potential distribution depends on the grain radius. It is clear that at a constant value of the surface potential of the dust grain the field at the surface decreases as the radius of the grain increases. This means that the fine grains are screened at shorter distances.

The following asymptotic relations can be written out for the solutions of Eq. (7) concerning the first derivative:

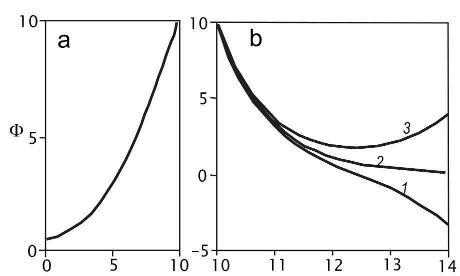

FIG. 2. Solutions of Eq. (7) for radius of grain $a=10r_D$. (a) Equation (11b); (b) line 2, Eq. (11c) or Eq. (11d), $\delta=0$; line 1, Eq. (11d), $\delta>0$; line 3, Eq. (11d), $\delta<0$.

$$\Phi' = \pm\exp\frac{\Phi}{2}[1+0(1)], \quad \Phi\to\infty, \tag{11a}$$

$$\pm\frac{1}{3}\sinh(\gamma)x[1+0(1)], \quad x\to 0, \tag{11b}$$

$$\pm\Phi\left(\frac{1}{x}+1\right)[1+0(1)], \quad x\to\infty, \quad \Phi\to 0, \tag{11c}$$

$$\pm\frac{x_0^2}{x^2}2\sqrt{\sinh^2\frac{\Phi}{2}+\delta}[1+0(1)], \quad x\to x_0, \tag{11d}$$

where γ is the value of the potential at the point $x=0$, and x_0 is an arbitrary point within the area of definition of the solution. The stationary value δ defines the view of dependence $\Phi(x)$: if $\delta>0$, the dependence looks like curve 1; if $\delta=0$, the dependence looks like curve 2; if $\delta<0$, the dependence looks like curve 3 in Figs. 1 and 2.

Let us compare Eq. (11a) to the expression for the field at a flat surface in a plasma:

$$\Phi' = 2\sinh\frac{\Phi}{2} = \exp\frac{\Phi}{2} - \exp\frac{-\Phi}{2} \tag{12}$$

It is easy to see that, at the surface potential $|\Phi_s|\gg 1$, Eq. (12) coincides with Eq. (11a). Hence the deduction, which is very important for the simplified description of the potential distribution around the grain, that at large values of the surface potential ($e|\phi_s|\gg T$) the curvature of the grain can be neglected, and the solution of the plane problem [11] can be used,

$$\Phi(x) = 2\ln\frac{1+\tanh(\Phi_s/4)\exp(a/r_D-x)}{1-\tanh(\Phi_s/4)\exp(a/r_D-x)}, \quad \Phi_s\gg 1. \tag{13}$$

Thus, we extend the applicability of Eq. (13), which was earlier used only for the obvious case of $a\gg r_D$.

The bulk plasma potential Eq. (6) in this case is described by the expression

$$\varphi_{pl} = -2\frac{T}{e}\tanh\frac{\Phi_s}{4}, \tag{14}$$

i.e., it defines a constant in Eq. (13).

Equation (11b) describes the distribution of the field in a restricted volume of the plasma, when there are no charged grains inside. In this case, the bulk plasma potential Eq. (6) is described by the expression

$$\varphi_{pl} \sim -\frac{T}{e}\sinh(\gamma)\frac{R^2}{15r_D^2}, \tag{15}$$

where R is the radius of the spherical volume.

The bulk plasma potential Eq. (15) grows proportionally to the surface area, restricting the volume of the plasma, as only the active surface is the source of volumetric charge in the plasma in this case.

Equation (11c) after integration coincides with the Debye potential $\Phi(x)=C\exp(-x)/x$; thus it describes the linearized Poisson-Boltzmann equation. Because on the boundary of the Wigner-Seitz cell $\phi(R_W)\sim\phi'(R_W)\sim 0$, the bulk plasma potential in this case is described by the expression

$$\varphi_{pl}\sim-\phi_s\left(\frac{1}{2}+\frac{r_D}{a}\right). \tag{16}$$

Equation (11d) is valid in the vicinity of Δx of any point x_0 belonging to the interval $[a,R]$, where R is the radius of the considered volume of plasma with the grain of radius a in the center. This equation can be reduced to the following form:

$$\int\frac{d\Phi}{2\sqrt{\sinh^2(\Phi/2)+\delta}}=\mp x_0^2\left(\frac{1}{x}-C(x_0)\right). \tag{17}$$

Equation (17) contains an integral which is the solution of the plane problem, i.e., the solution of the equation $\Phi''=\sinh(\Phi)$, which describes the potential in the plasma near the flat surface. It is possible to reduce this integral to a canonical form, by defining the limits of integration from the value Φ up to an infinitely large value and carrying out the replacement $t=\sinh(\Phi/2)$,

$$\int_\Phi^\infty\frac{dt}{\sqrt{(t^2+1)(t^2+\delta)}}=x-\lambda, \tag{18}$$

where λ is the value of coordinate at which the potential tends to infinity (it is clear that always $\lambda<a/r_D$).

The solutions of Eq. (18) are represented according to Ref. [25] in Jacobi elliptic functions, and are periodic functions with the period $4\mathbf{K}$, where $\mathbf{K}$ is the complete elliptic integral of the first kind:

$$\mathbf{K}(m)=\int_0^1\frac{dt}{\sqrt{(1-t^2)(1-mt^2)}}, \tag{19}$$

where $m=1-\delta$ for $\delta>0$ and $m=1/(1-\delta)$ for $\delta<0$.

This means that the solution reaches infinite values at a distance of $2\mathbf{K}$ from λ, i.e., the radius of the Wigner-Seitz cell $R_W=(4\pi N_d/3)^{-1/3}$ must satisfy the inequality

$$R_W/r_D<\mathbf{K}.$$

As it follows from the tables [25] for the complete elliptic integrals of the first kind, to large values of $\mathbf{K}$ there correspond values of the parameter $m\cong 1$. For example, to the value $\mathbf{K}=4$ there corresponds $m=0.995$, whence it follows that $\delta=\pm 0.005$. At such small values of the constant δ it can be neglected, i.e., in this case we can use the solution for a single grain in an infinite plasma, because at the distance of $4r_D$ the potential decreases from the infinitely large value up to the value $\phi\sim 0.1T/e$. Hence, if the Wigner-Seitz radius $R_W>4r_D$, it is always possible to use the boundary conditions $\phi(\infty)=0$, because the chosen grain does not feel influence of other grains.

Thus, the space-charge layer at the grain surface cannot exceed $4r_D$ in the flat case, and as the grain radius decreases it becomes even less. The number density of grains in the plasma is usually such that $R_W\gg r_D$. Therefore, the change of the charge of an individual grain does not affect the field at the surface of other grains, i.e., the grains do not interact via the electrical potential. Therefore, the forces responsible for observable ordering of grains in the plasma are not of electrical nature.

It is necessary to consider the bulk plasma potential Eqs. (14)–(16) in diagnosing the plasma as it defines the change of the chemical potential of electrons, $\delta\mu_e\cong-e\varphi_{pl}/2$; therefore, the measured value of the electrostatic potential depends both on the relative potential ϕ and on the bulk plasma potential [20].

IV. CONCLUSION

In the presented paper, we intentionally do not consider the range of validity of the Poisson-Boltzmann theory as this theory is applied in many fields of physics. Based on our analysis using it, it is possible to draw the following conclusions.

(i) The Poisson-Boltzmann equation in spherical symmetry has only four kinds of solution whose qualitative patterns are presented in the plots. The asymptotics of these solutions are described by Eqs. (11).

(ii) At large charges of the dust grain, the grain curvature can be neglected and it is possible to use the solution of the plane problem. Thus, the solution of the plane problem can be used for grains with large radius, when $a\gg r_D$, and under the condition of $|\phi_s|\gg T/e$ for grains of any radius. In this case, the plane solution is used immediately at the grain surface in the area of change of the potential $\infty>|\phi|\geq 1$, which corresponds to the maximal distance $1.4r_D$ [25]. Further, it is necessary to renormalize the potential as, for example, is done in Ref. [11] and transfer to the spherically symmetrical Debye potential.

(iii) The potential changes from a constant large value up to a value of $0.1T$ at the distance of $4r_D$ in the plane, and this distance decreases as the curvature of the grain surface increases. This means that the maximum distance where the field exists is $4r_D$, and as the grain radius decreases the screening effect increases. Thus, within the limits of the Poisson-Boltzmann theory, the electrical interaction between grains exists only at distances, smaller than $8r_D$.

[1] M. Knott and I. J. Ford, Phys. Rev. E **63**, 031403 (2001).
[2] K. S. Schmitz, Phys. Rev. E **65**, 061402 (2002).
[3] E. Trizac, L. Bocquet, and M. Aubouy, Phys. Rev. Lett. **89**, 248301 (2002).
[4] J. Dobnikar, M. Brunner, H. H. von Grünberg, and C. Bechinger, Phys. Rev. E **69**, 031402 (2004).
[5] V. E. Fortov, A. G. Khrapak, S. A. Khrapak, V. I. Molotkov, and O. F. Petrov, Phys. Usp. **174**, 495 (2004).

[6] D. H. E. Dubin and T. M. O'Neil, Rev. Mod. Phys. **71**, 87 (1999).
[7] P. M. Bellan, Phys. Plasmas **11**, 3368 (2004).
[8] M. Lampe, G. Joyce, G. Ganguli, and V. Gavrishchaka, Phys. Plasmas **7**, 3851 (2000).
[9] T. Bystrenko and A. Zagorodny, Phys. Lett. A **299**, 383 (2002).
[10] F. Verheest, V. V. Yaroshenko, and M. Helberg, Phys. Plasmas **9**, 2479 (2002).
[11] I. T. Yakubov and A. G. Khrapak, Sov. Technol. Rev. B **2**, 269 (1989).
[12] M. E. Markes and P. F. Williams, Phys. Lett. A **278**, 152 (2000).
[13] S. V. Vladimirov and N. F. Cramer, Phys. Rev. E **62**, 2754 (2000).
[14] P. K. Shukla, Phys. Plasmas **8**, 1791 (2001).
[15] M. K. Mahanta and K. S. Goswami, Phys. Plasmas **8**, 665 (2001).
[16] A. P. Nefedov, O. F. Petrov, V. I. Molotkov, and V. E. Fortov, JETP Lett. **72**, 218 (2000).
[17] J. Vranješ, M. Y. Tanaka, B. P. Pandey, and M. Kono, Phys. Rev. E **66**, 037401 (2002).
[18] E. G. Gibson, Phys. Fluids **2**, 2389 (1966).
[19] V. I. Vishnyakov and G. S. Dragan, Phys. Rev. E **74**, 036404 (2006).
[20] V. I. Vishnyakov and G. S. Dragan, Phys. Rev. E **71**, 016411 (2005).
[21] V. I. Vishnyakov and G. S. Dragan, Phys. Rev. E **73**, 026403 (2006).
[22] V. M. Evtuhov, Bull. Acad. Sci. Georgian SSR **106**, 473 (1982).
[23] V. M. Evtuhov, Math. Nachr. **115**, 215 (1984).
[24] B. V. Deryagin, Kolloid-Z. **16**, 425 (1954).
[25] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun Natl. Bur. Stand. Appl. Math. Ser. No. 5, (U.S. GPO, Washington, D.C., 1964).