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HEURISTIC SOLUTION OF LANGMUIR PROBLEM IN ARBITRARY DOMAIN

The Langmuir problem for a collisionless plasma was formulated and solved for some simple domains at 1921. But, for more complicated cases, no robust method is known till now except for the macro particle simulation. We propose a new method applicable to domains with arbitrary boundary shape. The method is based on the solution of the well-known eigenvalue problem for diffusion-type equations. The comparison of test solutions obtained by this technique with the Particle-In-Cell method demonstrates an acceptable accuracy despite the lack of theoretical validation of this method.

K e y w o r d s: collisionless plasma, Langmuir problem, free fall regime.

1. Statement of the Problem

There are a great variety of low temperature gas discharge technological devices operated under low pressures. If we have a steady-state plasma with Maxwellian electrons and ions with mean free path greater than the plasma size, then the problem can be considered as the Langmuir one [1]. It is known that the solution of the Langmuir problem meets considerable difficulties, if the chamber shape differs from a flat layer, cylinder, or sphere. So, we were able to indicate the only work [2] devoted to the analytical treatment of the free-fall motion of ions in an arbitrary 3D domain. Another approach to the problem is to use fluid equations to model the collisionless ion motion. In [3–5], the one-dimensional fluid equation was used to study a sheath-plasma region. In [6] a 2D fluid equations in the magnetized plasma was spatially averaged along magnetic field lines. However, these papers are devoted to the plasma sheath problem, and their results do not allow one to solve the problem in a 3D geometry. In this paper, we are focused on the plasma volume rather than a sheath.

For a low-pressure plasma, the macro particle methods (for example, the Particle-In-Cell or PIC one) [7, 8] are widely used. The corresponding software is freely distributed in many cases. However, these methods demand a lot of computational resources, especially with decrease in the Debye radius. Therefore, it would be helpful to find some less resource-consuming method for calculations of the collisionless plasma density.

There are quite simple codes based on the diffusion model of transport of particles in a gas discharge plasma (see, e.g., [10]). However, they are invalid in the range of low gas pressures. The diffusion coefficient tends to infinity as the frequency of ion-neutral collisions tends to zero, and the solution with constant ion density can be obtained in this case. This is all the more regrettable, because the solvers of elliptic equations are fast, precise, and easy for coding.

The main idea of the approach proposed in this paper is to apply the diffusion equations with specifically tailored diffusion coefficient. We demonstrate a variant of such tailoring that allows us to construct a boundary-value problem for elliptic partial differential equations (PDE) with a solution rather close to the exact collisionless solution. The results obtained

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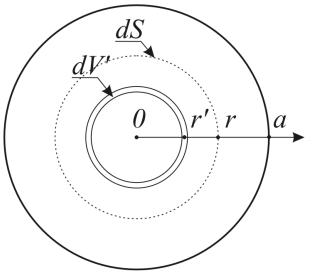

Fig. 1. Cylinder configuration in the Langmuir problem

within this approach are compared with those obtained by the PIC method described in [8,9]. It should be mentioned that the proposed approach gives a nonstrict but rather heuristic solution of the problem.

The plan of our speculative considerations is the following:

- calculation of the diffusion coefficients in the diffusion equations so that the solutions coincide with Langmuir ones for three 1D geometries;
- development of a method suitable for the extension of these 1D results to an arbitrary 3D domain.
- verification of the method by a PIC simulation.

2. Langmuir Solutions

In [1], L. Tonks and I. Langmuir had obtained the analytical solution for the plasma density in collisionless plasma layer, cylinder, and sphere. It would be useful to make a brief review of the solution. In Fig. 1, the cylinder of radius a filled with an ion-electron plasma is shown. Let the electron temperature T and the ionization frequency $\nu_i(T)$ be constant in the plasma, and let the quasineutrality condition be satisfied ($n_e \approx n_i \approx n$) at any point of the plasma volume. Here, n_e, n_i, and n are the densities of electrons, ions and plasma, respectively. Electrons obey the Boltzmann distribution, so

$$n(r) = n_0 \exp\left(e\varphi(r)/T\right), \tag{1}$$

where n_0 is the plasma density on the discharge axis, $\varphi(r) \leq 0$ is the ambipolar potential, and e is the elementary charge. Ions are accelerated by the ambipolar field along radial trajectories from the bearing points. From the ion liquid continuity equation, we can state that the ion source in the volume dV' contributes to the ion density at some point $r > r'$:

$$dn(r) = \frac{\nu_i n(r')\, dV'}{S(r)\sqrt{2e(\varphi(r') - \varphi(r))/M}}. \tag{2}$$

Here, M is the ion mass, and $S(r) = 2\pi r^2$. The total ion density $n(r)$ can be found by the dn integration over all sources in the interval $0 < r' < r$. With the use of (1), we obtain the integral equation for the ion density in the bulk plasma:

$$r \exp\left(e\varphi(r)/T\right) = \int_0^r \frac{\nu_i \exp\left(e\varphi(r')/T\right)}{\sqrt{2e(\varphi(r') - \varphi(r))/M}} r'dr'. \tag{3}$$

Let us introduce the normalized coordinate ξ and the normalized potential η by

$$\xi = r\frac{\nu_i}{u_{\rm B}}, \tag{4}$$

$$\eta = -\frac{\varphi}{T_e}, \tag{5}$$

where $u_{\rm B} = \sqrt{2T_e/M}$ is the Bohm velocity. In these variables, the solution of (3) is expressed as follows:

$$n = n_0 e^{-\eta}, \tag{6}$$

$$\xi = \sqrt{\eta}\sum_{m=0}^{\infty} a_m \eta^m. \tag{7}$$

One can obtain the same expansions for a sphere or flat layer, so the coefficients a_m depend on the boundary shape. It appears that the gradients of the potential η and density n tend to infinity, when ξ tends to a certain value ξ_0. This coordinate value is interpreted as the plasma-wall boundary (if the sheath region is negligibly small). We have

$$\left.\frac{d\xi}{d\eta}\right|_{\eta_0} = 0, \quad \xi_0 = \xi(\eta_0). \tag{8}$$

The electron temperature can be found from

$$\xi_0 = r_0\frac{\nu_i(T)}{u_{\rm B}(T)} \tag{9}$$

with the chamber radius r_0, value ξ_0, and dependence $\nu_i(T)$ being given.

3. Construction of the Diffusion Coefficient $\bar{D}$

We start from the 1D Langmuir problem and introduce a function $\bar{D}(\xi)$ satisfying the equation

$$-\frac{1}{\xi^\alpha}\frac{d}{d\xi}\xi^\alpha \bar{D}\frac{dn}{d\xi} + n = 0, \tag{10}$$

where $\xi \in (0, \xi_0)$. Here, $\alpha = 0, 1, 2$ for the flat, cylindrical, and spherical cases, respectively, and $n(\xi)$ is determined by (6)–(7). Then the normalized ion flux density

$$j(\xi) = -\bar{D}\frac{dn}{d\xi} = \frac{1}{\xi^\alpha}\int\limits_0^\xi n(\xi')\,\xi'^{\,\alpha} d\xi', \tag{11}$$

and

$$\bar{D}(\xi) = -j\,\frac{d\xi}{dn}. \tag{12}$$

Figure 2 illustrates the calculated dependences of the density, flux, and diffusion coefficient on ξ and shows that

$$-j(\xi_0) \approx n(\xi_0) \tag{13}$$

at the boundary ξ_0.

We consider the approximate equality (13) as the exact one and impose the boundary condition

$$\bar{D}\frac{dn}{d\xi} + n\big|_{\xi_0} = 0 \tag{14}$$

on Eq. (10) to obtain the boundary-value problem. At least one solution of (10), (14) would coincide with the exact Langmuir solution, if equality (13) is strict. But (10), (14) has a nonzero solutions only for a certain value ξ_0. It is therefore natural to reformulate (10), (14) as the eigenvalue problem. Let the segment $\xi \in (0, \xi_0)$ can be obtained from an arbitrary segment $r \in (0, r_0)$ by

$$\xi = \sqrt{\mu}\, r, \tag{15}$$

where μ is an unknown constant. Expressions (10)–(14) pass to

$$\frac{1}{r^\alpha}\frac{d}{dr} r^\alpha \bar{D}(\sqrt{\mu}\, r)\frac{dn}{dr} + \mu\, n = 0, \tag{16}$$

$$\bar{D}(\sqrt{\mu}\, r)\frac{dn}{dr} + \sqrt{\mu}\, n\big|_{r_0} = 0. \tag{17}$$

One of the harmonics of the spectrum of this nonlinear eigenvalue problem "nearly" coincides with the exact Langmuir solution (the deviation is caused only by (13)). It is reasonable to consider the fundamental harmonic as this one, because the plasma density does not tend to zero.

Relations (9) and (15) yield the following expression to determine the temperature:

$$\sqrt{\mu} = \frac{\nu_i(T)}{u_{\rm B}(T)}. \tag{18}$$

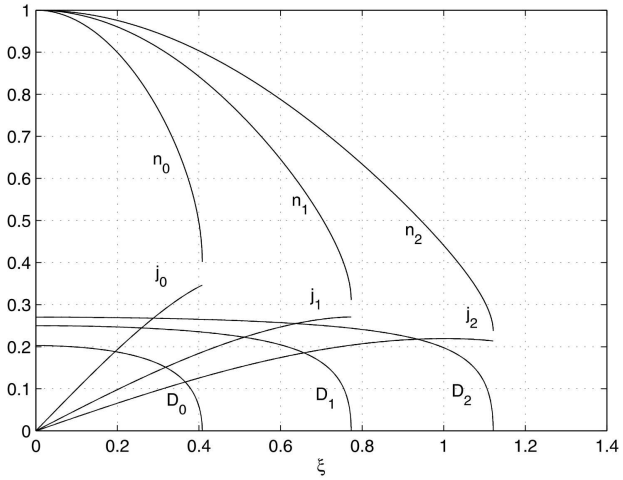

Fig. 2. Dependences $n_\alpha(\xi)$, $|j_\alpha(\xi)|$, and $D_\alpha(\xi)$ for $\alpha = 0, 1, 2$

Relations (16)–(17) cover all the domains Ω_m with the same shape, but with different sizes $r_{0,m}$. The corresponding eigenvalues $\sqrt{\mu_m}$ are the such that

$$\sqrt{\mu_1} r_{0,1} = \sqrt{\mu_2} r_{0,2} = ... = \xi_0. \tag{19}$$

So, since the diffusion coefficients depend on the coordinate r_m as $\bar{D}(\sqrt{\mu_m} r_m)$, all the distributions of the $\bar{D}$ over the corresponding domains Ω_m are the same:

$$\bar{D}(r_1) = \bar{D}(r_2) = ... \tag{20}$$

The diffusion coefficient $\bar{D}$ still depends on α. Now, we will try to make this dependence implicit by expressing $\bar{D}$ via a certain variable, which must be determined for arbitrary flat layers, cylinders, and spheres in some uniform manner.

Due to (14), the equality $\bar{D}(r) = 0$ should be satisfied on the boundaries, because the density gradient tends to infinity, whereas the ion flux is fixed. This suggests that $\bar{D}$ depends on the solution f of the eigenvalue problem. Let us consider that

$$\frac{1}{r^\alpha}\frac{d}{dr}\, r^\alpha \frac{df}{dr} + \lambda f = 0, \tag{21}$$

$$f|_{\partial\Omega} = 0, \tag{22}$$

where f is the main harmonic of the problem, and λ is the corresponding eigenvalue. We will normalize f so that $\max(f) = 1$ in order that $\bar{D}(f)$ be consistent with condition (20).

One can see from Fig. 3 that $\bar{D}$ takes one of three different values at the certain f depending on α

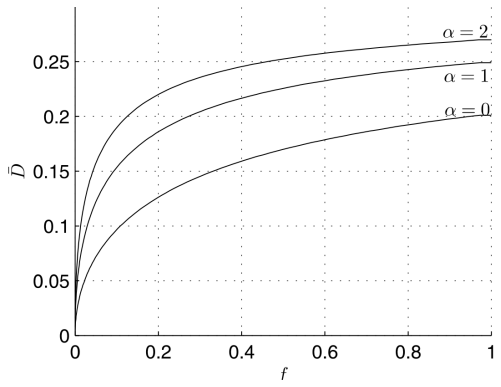

Fig. 3. $\bar{D}$ versus the normalized eigenfunctions f for a layer, cylinder, and sphere

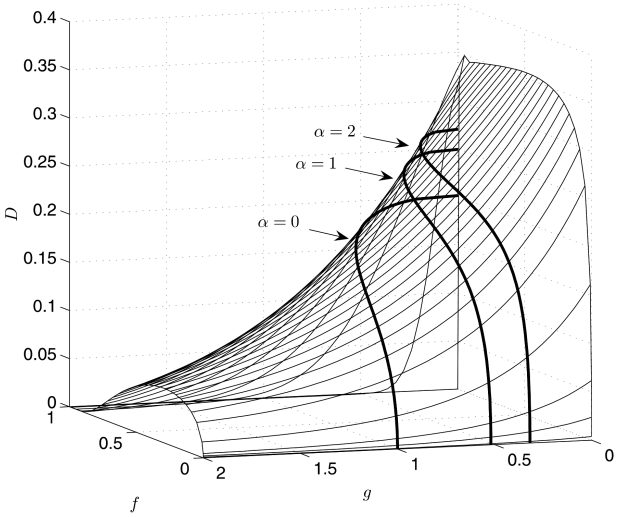

Fig. 4. Curves of $\bar{D}(f, g)$ for a layer, cylinder, and tailoring surface built by (25)

and, therefore, cannot depend on f only. Let us consider the derivative $g = |df/(dr\sqrt{\lambda})|$ along with f, which is a linearly independent function. The curves $\bar{D}(f, g)$ for $\alpha = 1, 2, 3$ are presented in Fig. 4. If we interpolate in between and extrapolate outside of these curves, we can expect to obtain $\bar{D}$ for any domain. Such approximation must obey the following conditions:

$$\bar{D}(f, g) \underset{g\to\infty}{\longrightarrow} 0, \tag{23}$$

$$\bar{D}(0, g) = 0. \tag{24}$$

We approximate $\bar{D}(f, g)$ as follows:

$$\bar{D}(f, g) = a(f)\, \exp\left(-g\left(p(f)\, g + q(f)\right)\right). \tag{25}$$

The coefficients $a(f)$, $p(f)$, and $q(f)$ are chosen so that $\bar{D}(f, g)$ takes correct values for all three 1D problems (see Fig. 3).

It should be emphasized that the approximation of the diffusion coefficient could be done in many different ways. In order to choose the optimal form of the approximation, we tried numerous variants. The verification has shown that (25) provides the lowest deviation from PIC simulation results.

4. Algorithm

Let us consider the main idea of obtaining the solution in an arbitrary 3D domain. The problem is formulated by analogy with (16)–(17):

$$\nabla\bar{D}\nabla n + \mu n = 0, \tag{26}$$

$$\mathbf{N}\bar{D}\nabla n + \sqrt{\mu}n\big|_{\partial\Omega} = 0. \tag{27}$$

The domain Ω is the volume filled with a plasma, amd the vector $\mathbf{N}$ is the outer boundary normal of the domain Ω. The eigenvalue μ is unknown. Due to the nonlinear boundary condition, we propose the following iteration process:

$$\nabla\bar{D}\nabla n + \mu_j n = 0, \tag{28}$$

$$\mathbf{N}\bar{D}\nabla n + \sqrt{\mu_{j-1}}n\big|_{\partial\Omega} = 0, \tag{29}$$

where j is the iteration number. In the first iteration ($j = 1$), we assume $\mu_0 = 1$ in the boundary condition and obtain the eigenvalue μ_1 by solving of the linear eigenvalue problem. In the second iteration ($j = 2$), we fix μ_1 in the boundary condition and obtain the next approximation to the eigenvalue, μ_2, and so on. Iterations stop when the deviation $|\mu_j - \mu_{j-1}|$ is small enough. This scheme converges readily for any initial μ.

The diffusion coefficient is calculated by (25). The variables f, g are found only once from the main harmonic f of the boundary-value problem:

$$\triangle f + \lambda f = 0, \tag{30}$$

$$f|_{\partial\Omega} = 0, \tag{31}$$

$$\max(f) = 1, \tag{32}$$

$$g = |\nabla_{r\sqrt{\lambda}} f|. \tag{33}$$

The discharge temperature can be obtained from (18).

5. Results and Discussion

The comparison of the results using the described method with the PIC method with Monte-Carlo collisions [8, 9] was performed for the verification. The ICP discharge in argon at a pressure of 0.2 mTorr sustained in the cylindrical chamber with a radius of 10 cm and a height of 20 cm was simulated. The 2D simulation in cylindrical coordinates was performed on a 100×100 uniform rectangular grid. The equilibrium electron temperature was 8 eV, the time steps were 10^{-10} s for electrons and 10^{-8} s for ions. The neutral gas temperature was set to be 0.03 eV. One macroparticle contained 2×10^6 particles. The total number of macroparticles was up to 5×10^5.

The discrepancy between the solutions was about 1% inside the domain and reach 5% at the boundary. In order to test our method with more complicated boundary shapes a diaphragm or a needle were placed inside. The diaphragm is perpendicular to the cylinder axis (Fig. 5), and the needle is placed along the cylinder axis (Fig. 6). Plasma density distributions obtained by these methods are shown in Figs. 5, 6. The distributions are normalized to the maximal value. Generally, the heuristic method gives the density values less than the PIC method does. The deviation is $\lesssim$5% inside the domain and reaches maximal value on the domain boundary. The worst deviation up to $\sim$70% appears only in a little region near the needle tip.

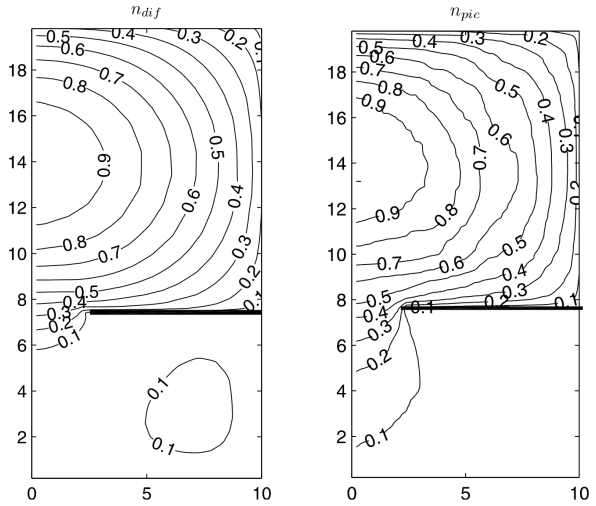

Fig. 5. Plasma density distributions in a cylinder with diaphragm: obtained by the heuristic method ($n_{\rm dif}$) and by the PIC method ($n_{\rm pic}$)

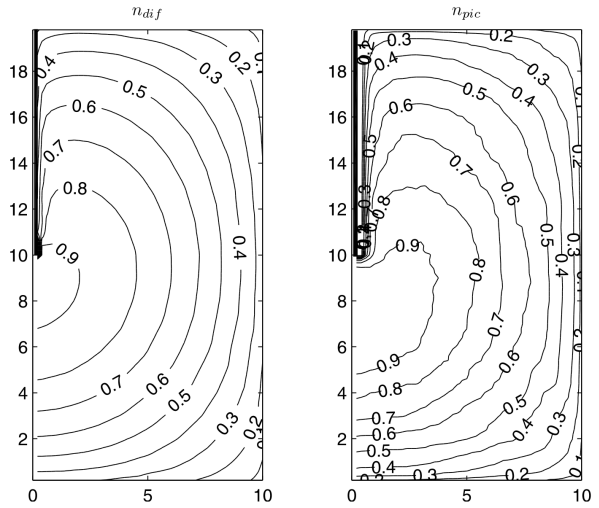

Fig. 6. The same as in Fig. 5 for a cylinder with needle

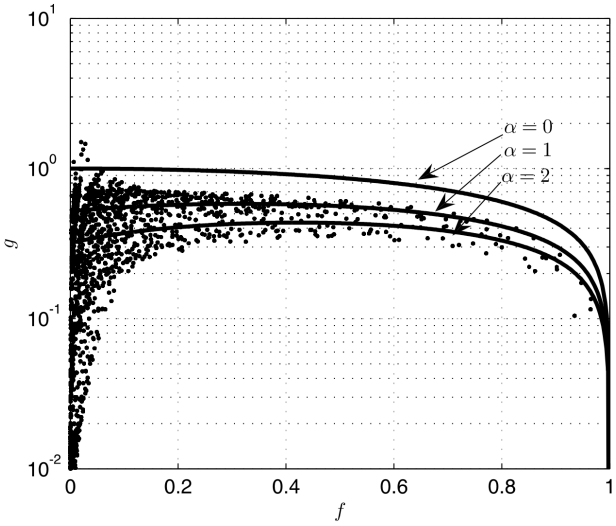

Fig. 7. Points (f, g) where $\bar{D}(f, g)$ was calculated; for the configuration in Fig. 5

The calculation of $\bar{D}$ is performed at the nodes of a triangular grid built for a numerical solution of the diffusion equation and demands the definition of a pair (f_i, g_i) at each node i. The distribution of the points (f_i, g_i) is shown in Figs. (7)–(8) together with the curves $f(g)$ for 1D solutions. We conclude that large deviations of the density are caused by extrapolation errors and arise near the boundary, where the derivative values are high enough, and the nonstrict condition (13) is used.

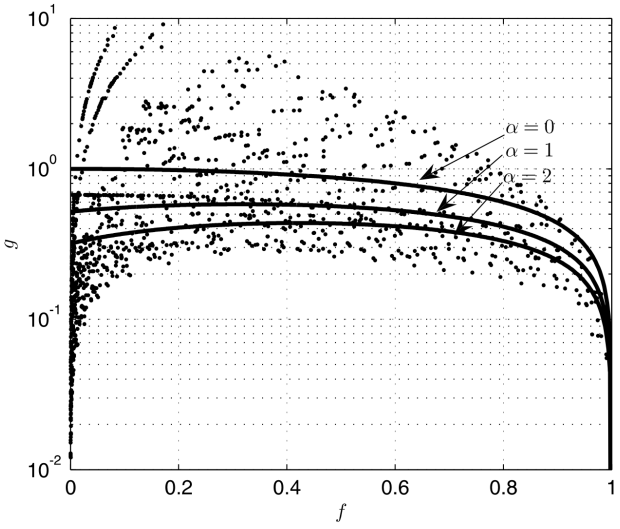

Fig. 8. The same as in Fig. 7 for the configuration in Fig. 6

The electron temperature has been found from (18) and is less than the temperature obtained within the PIC method by 10–15%, while the ionization frequency $\nu_i(T)$ is the same in both cases.

6. Conclusion

In this paper, we have formulated the task of reducing the 3D Langmuir problem in an arbitrary domain to the boundary value problem for diffusion-type equations. We have proposed a heuristic method of such transformation based on the diffusion coefficient tailoring. The verification of the method by the comparison of the results with those of a PIC simulation shows a satisfactory accuracy for the enough complicated domains. Thus, the method can be used for the plasma simulation in industrial devices. At the same time, the mathematical justification of the described method requires a further research.

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ЕВРИСТИЧНИЙ РОЗВ'ЯЗОК
ЗАДАЧІ ЛЕНГМЮРА В ДОВІЛЬНІЙ ОБЛАСТІ

Р е з ю м е

Задачу Ленгмюра для плазми без зіткнень було сформульовано та розв'язано для деяких простих областей у 1921 р., але для складніших випадків досі немає ефективних методів за винятком прямого моделювання. Ми пропонуємо новий метод, що можна застосувати для областей довільної форми. Метод оснований на розв'язку добре відомих задач на власні значення для рівнянь дифузійного типу. Порівняння тестових розв'язків з отриманими методом частинок у комірках показало прийнятну точність, незважаючи на брак теоретичного обґрунтування методу.