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The Evolution of the Charge Density Distribution Function for Spherically Symmetric System with Zero Initial Conditions

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ABSTRACT

The evolution of the charge density distribution function is simulated for both the case of a uniformly charged sphere with zero initial conditions and for the case of a non-uniform charged sphere. For the case of a uniformly charged sphere, the comparison of a numerical result and an exact analytical solution, demonstrated the agreement between the results. The process of "scattering" of a charged system under the influence of its own electric field has been illustrated on the basis of both the particle-in-cell method and the solution of the Cauchy problem for vector functions of the electric field and vector velocity field of a charged medium.

KEYWORDS

Charge Density Distribution; Cauchy Problem; Non-Uniform Charged Sphere; Particle-in-Cell

1. Introduction

The methods developed in non-equilibrium statistical mechanics [1-3] are effectively applied while considering different problems connected with the behavior of the systems of various charged particles. Such is the case for consideration of the influence of the beam's own electric field on the evolution of the charge density distribution function. Now, as the number of problems with an exact solution is not that big, different numerical methods have been widely disseminated [4,5]. A certain set of parameters is used during the simulation, and therefore it is important to specify a path to perform physical problem adequacy testing of such a modeling approach. The example of such testing can be a comparison of the simulation results for a given set of parameters and the results drawn on the basis of an exact solution of a theoretical problem.

In this paper, we consider the Cauchy problem for the evolution of the charge density distribution function for a spherically symmetric system with zero initial conditions for the velocity field $\boldsymbol{v}(p,t)$ and nonzero initial conditions for the electric field vector $\boldsymbol{D}(p,t)$.

$$\begin{cases} \boldsymbol{D}_t(p,t)+\boldsymbol{v}(p,t)\cdot \operatorname{div}\boldsymbol{D}(p,t)=0, \quad p\in\Omega \\ \boldsymbol{v}_t(p,t)+\left(\boldsymbol{v}(p,t),\nabla\right)\boldsymbol{v}(p,t)=\dfrac{\alpha}{\varepsilon_0}\boldsymbol{D}(p,t) \\ \boldsymbol{D}\big|_{t=0}=\boldsymbol{D}_0(p), \quad \boldsymbol{v}\big|_{t=0}=\boldsymbol{\Theta} \end{cases} \tag{1}$$

where $(\boldsymbol{a},\boldsymbol{b})$ denotes the scalar product of vectors $\boldsymbol{a}$ and $\boldsymbol{b}$; ∇ denotes the nabla differential operator; ε_0 denotes the dielectric constant of the vacuum and $\boldsymbol{\Theta}$ denotes zero initial velocity vector. The variable p corresponds to spatial coordinates (x,y,z), and the variable t represents time. The constant $\alpha=q/m$ sets the ratio between the charge and the mass of the particles. Ω represents the area in which the solution of the system is being considered. This system, together with the initial conditions, leads to the formulation of the Cauchy problem (1), the solution of which describes the evolution of

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the charge density distribution function under the influence of its own electric field.

It should be noted that the Cauchy problem (1) has an exact solution for the uniformly charged sphere, which has the form

$$t = \frac{R_0^{3/2}}{\sqrt{2\gamma}}\left(\sqrt{\left(\frac{\rho_0}{\rho}\right)^{1/3}\left(\left(\frac{\rho_0}{\rho}\right)^{1/3}-1\right)}+\frac{1}{2}\operatorname{arcch}\left(2\left(\frac{\rho_0}{\rho}\right)^{1/3}-1\right)\right) \quad (2)$$

where R_0 is the initial radius of the sphere; ρ_0 is the initial charge density in the sphere; the constant $\gamma = \frac{\alpha Q}{4\pi\varepsilon_0}$, where Q is the total charge of the sphere. The function $\rho(t)$ indicates the charge density in the sphere at the moment of time t, which is associated with the electric field vector $\boldsymbol{D}(p,t)$ by Maxwell's equation $\operatorname{div}\boldsymbol{D} = \rho$.

2. Approximation of the Solution

The solution of the problem (1) may be found in the form of expanding vector functions of the electric field $\boldsymbol{D}(p,t)$ and vector functions of the velocity field $\boldsymbol{v}(p,t)$ into series:

$$\begin{aligned}\boldsymbol{D}(p,t) &= \boldsymbol{D}(p,0)+t\cdot\boldsymbol{D}_t(p,0)+\frac{t^2}{2}\boldsymbol{D}_{tt}(p,0)+\cdots \\ &= \sum_{k=0}^{\infty}\frac{\partial^k \boldsymbol{D}}{\partial t^k}(p,0)\frac{t^k}{k!} \\ \boldsymbol{v}(p,t) &= \boldsymbol{v}(p,0)+t\cdot\boldsymbol{v}_t(p,0)+\frac{t^2}{2}\boldsymbol{v}_{tt}(p,0)+\cdots \\ &= \sum_{k=0}^{\infty}\frac{\partial^k \boldsymbol{v}}{\partial t^k}(p,0)\frac{t^k}{k!}\end{aligned} \quad (3)$$

where the expansion coefficients in (3) can be expressed in terms of the derivatives of the initial conditions of the problem (1). Therefore, for the numerical solution of the problem (1), the approximation of the first two terms of the series (3) is to be considered. That is, for each time step, the approximation of the solution is obtained in the form of:

$$\begin{aligned}\boldsymbol{D}(p,t_{n+1}) &\approx \boldsymbol{D}(p,t_n)+\tau\cdot\boldsymbol{D}_t(p,t_n) \\ \boldsymbol{v}(p,t_{n+1}) &\approx \boldsymbol{v}(p,t_n)+\tau\cdot\boldsymbol{v}_t(p,t_n)\end{aligned} \quad (4)$$

where $n = 0,1,\cdots,N$; N is the total number of time steps; τ is the step in the time t. The coefficients of the time τ in the first power are expressed in terms of the derivatives of $\boldsymbol{D}$ and $\boldsymbol{v}$ of the previous step in time t_n by formulas:

$$\begin{aligned}\frac{\partial \boldsymbol{D}}{\partial t}(p,t_n) &= -\boldsymbol{v}(p,t_n)\cdot\operatorname{div}\boldsymbol{D}(p,t_n) \\ \frac{\partial \boldsymbol{v}}{\partial t}(p,t_n) &= -(\boldsymbol{v}(p,t_n),\nabla)\boldsymbol{v}(p,t_n)+\frac{\alpha}{\varepsilon_0}\boldsymbol{D}(p,t_n)\end{aligned} \quad (5)$$

As a result, the formulas (4), (5) can be used for the numerical solution of the problem (1).

3. An Example of the Numerical Solution

Let's perform a numerical simulation of the Cauchy problem (1). For this we solve the Cauchy problem (1) in two ways: by using the difference Schemes (4-5) and by using the PP (Particle-to-Particle) method. The results are compared with the known analytical solution (2).

So, due to the symmetry of the problem we use a spherical coordinate system.

We write the initial conditions for the case of a uniformly charged sphere:

$$\begin{aligned}&\boldsymbol{v}\big|_{t=0} = \boldsymbol{\Theta},\quad \boldsymbol{D}_0(r) = \boldsymbol{e}_r\frac{\rho_0}{3}r,\quad r\in[0,R_0] \\ &\rho_0 = \frac{Q}{V},\quad Q = N_p q,\quad V = \frac{4}{3}\pi R_0^3 \\ &R_0 = 2м,\quad N_R = 200,\quad T = 0.1c \\ &N_p = 2000,\quad N_T = 200\end{aligned} \quad (6)$$

here we use the following notations: V is the initial volume of the sphere; N_p is the number of large particles for the simulation using PP (Particle-to-Particle) method; q is the charge of one particle-in-cell; N_R is the number of computational mesh nodes along the radius; T is the time interval during which the evolution of the system occurs; N_T is the number of time steps.

The numerical results are shown in **Figures 1(a)** and **(b)**. **Figure 1(a)** shows the distribution of the charge density $\rho(r)$ along the radius. The solid line shows the distribution of the charge density, which corresponds to the problem (1). The bar chart shows the result which corresponds to PP method. The graphs shown in the figure represent the initial and final time. The dotted line shows the theoretical solution obtained by the formula (2). **Figure 1(b)** shows the graphs of $\rho(r)r^2$ **Figure 1(b)** presents the distribution of the linear density along the radius, and shows the conservation of the curvilinear trapezoidal area, which corresponds to the total charge Q.

The graphs in **Figures 1(a)** and **(b)** show that the difference scheme in Equations (4) and (5) has a good agreement with the theoretical result. To illustrate the results obtained by PP method, the bar chart is used. At the origin, with a radius equal to zero the approximation of the density function in the form of the bar chart has a characteristic feature in the graph: it shows the oscillation of the density function. This is due to the fact that if we want to

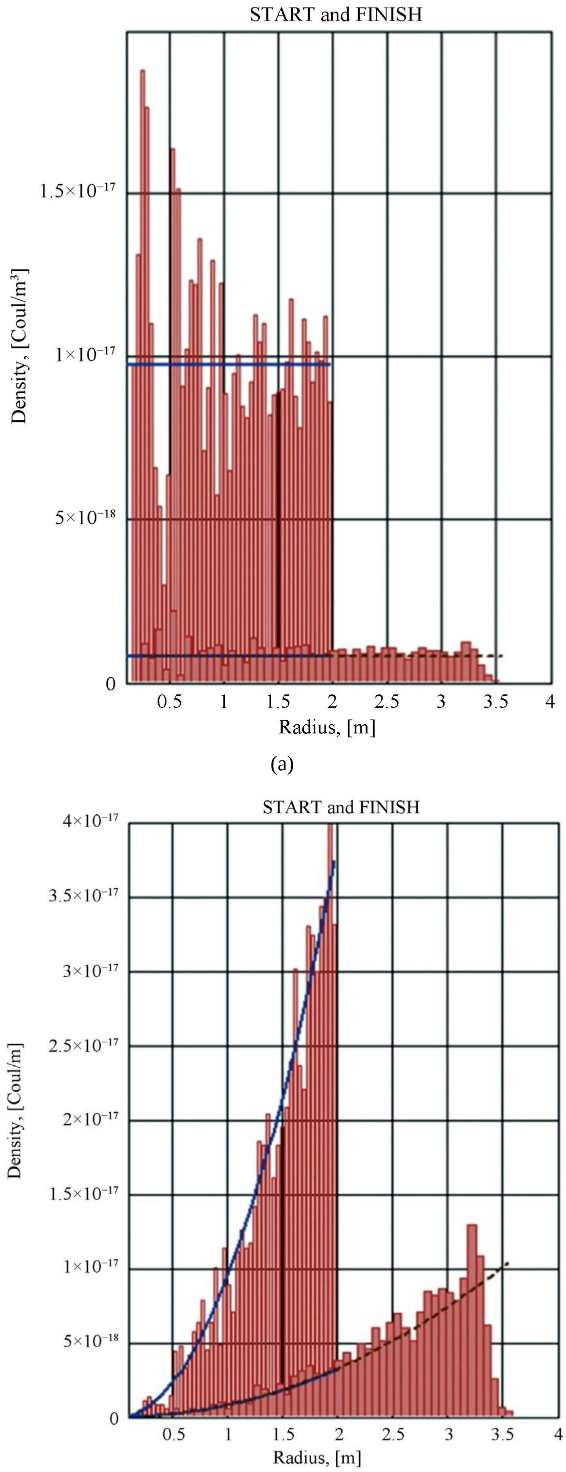


Figure 1. The initial and the final distribution of the charge density for a uniformly charged sphere.

determine the charge density we need to divide two small quantities—charge by volume. They are small quantities because while moving to the origin, and with the decreasing radius, the volume of the spherical layer or the sphere decreases. Consequently, the amount of charge contained in such volume must also decrease because the charge density is constant. Thus, at short distances the graph has a characteristic feature in the form of oscillation. This is due to the large error in the bar chart of the charge density function in the numerical generation of particle coordinates for PP method.

Figure 2 shows the evolution of the charge density distribution function. The solid line shows the theoretical graph and the dotted line shows the graph obtained numerically. It should be noted that the solution (2) doesn't depend on the coordinates, only on time. Therefore, at every time step within the sphere the density is independent of the radius and remains constant, *i.e.*, it depends only on time. Therefore, in **Figure 2** there is no dependence on the coordinates, *i.e.* the value of density can correspond to any point within the sphere. As follows from the graph in **Figure 2** there is a good agreement between the theory and the numerical solution obtained by the schemes in Equations (4) and (5), which has a first order approximation in time.

Figure 3 shows the configuration space for PP (Particle-to-Particle) method. On the left we can see the distribution of the particles at the initial time, and on the right—the final position of the particles. The figure shows the volumetric expansion of the sphere.

Let us analyze the behavior of the system of charged particles in the case of a non-uniform charge density. Let us consider a charged sphere with charge density distribution function in the form of:

$$\rho_n(r)=\frac{1}{\sqrt{2\pi}\sigma r}e^{-\frac{(\ln(r)-\mu)^2}{2\sigma^2}},\ \rho(r)=\frac{q}{2\pi r^2}N_p\rho_n(2r),\quad (7)$$

where $\rho_n(r)$ is a normal logarithmic distribution; σ,μ are constants. As initial conditions, we take the following values:

$$N_p=1000,\quad \mu=0,\quad \sigma=0.2\,м$$

$$\boldsymbol{V}_0(t)=\boldsymbol{\Theta},\quad \boldsymbol{D}_0(r)=\frac{\boldsymbol{e}_r}{r^2}\int_0^r s^2\rho(s)\mathrm{d}s \quad (8)$$

$$r\in[0,1]\,м,\quad N_R=200,\quad T=0.01\,c,\quad N_T=400$$

The solution of the problem will be sought in two ways: by the numerical solution of the Cauchy problem (1) using the algorithm (4-5) and by the PP (Particle-to-Particle) method. At the end of the calculations the two results are compared.

Suppose there is a three-dimensional area in which the problem is to be solved. To define the area, we take a parallelepiped with side lengths $L_{x_s},\ s=1,2,3$ as the geometric shape of the area. In this area we set a rectan-

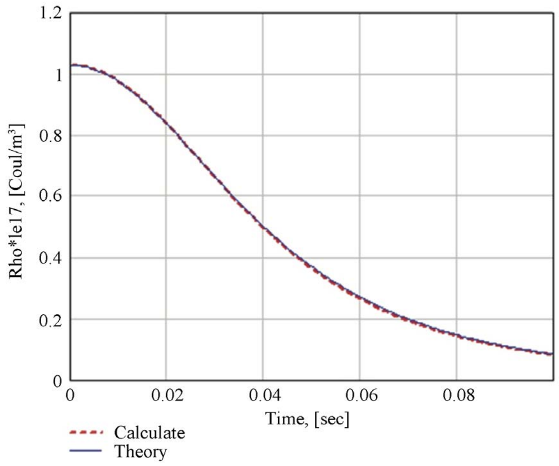


Figure 2. The evolution of the charge density distribution function for a uniformly charged sphere.

gular mesh

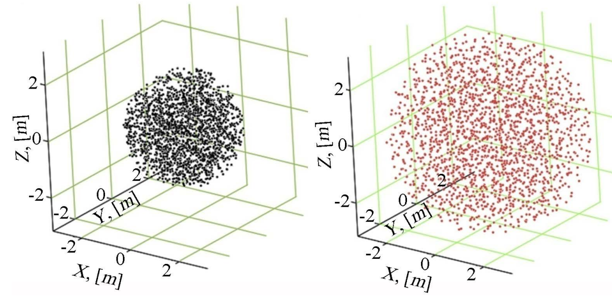
$$\{i,j,k\}=\left\{1\le i\le N_{x_1}-1, 1\le j\le N_{x_2}-1, 1\le k\le N_{x_3}-1\right\} \tag{9}$$

in increments of $h_{x_s}=\dfrac{L_{x_s}}{N_{x_s}}$, where N_{x_s} is the number of partitions of L_{x_s}. We set a time mesh $0\le n\le N_T-1$ in increments of $\tau=T/N_T$, where T is a period of time, in which the problem is to be solved. The system of difference equations (4) takes on the form:

$$\begin{aligned}
&D^{(x_s)}_{i,j,k,n+1}=D^{(x_s)}_{i,j,k,n}-\tau\rho_{i,j,k,n}V^{(x_s)}_{i,j,k,n},\\
&(x_1,x_2,x_3)\in R^3,\ s=1,2,3\\
&V^{(x_s)}_{i,j,k,n+1}=V^{(x_s)}_{i,j,k,n}+\tau\left(\frac{\alpha}{\varepsilon_0}D^{(x_s)}_{i,j,k,n}-dV^{(x_s)}_{i,j,k,n}\right)\\
&\rho_{i,j,k,n}=\frac{D^{(x_1)}_{i+1,j,k,n}-D^{(x_1)}_{i-1,j,k,n}}{2h_{x_1}}\\
&\qquad+\frac{D^{(x_2)}_{i,j+1,k,n}-D^{(x_2)}_{i,j-1,k,n}}{2h_{x_2}}+\frac{D^{(x_3)}_{i,j,k+1,n}-D^{(x_3)}_{i,j,k-1,n}}{2h_{x_3}}\\
&dV^{(x_s)}_{i,j,k,n}=V^{(x_1)}_{i,j,k,n}w1^{(x_s)}_{i,j,k,n}+V^{(x_2)}_{i,j,k,n}w2^{(x_s)}_{i,j,k,n}+V^{(x_3)}_{i,j,k,n}w3^{(x_s)}_{i,j,k,n}
\end{aligned} \tag{10}$$

where the expressions $w1^{(x_s)}_{i,j,k,n}, w2^{(x_s)}_{i,j,k,n}, w3^{(x_s)}_{i,j,k,n}$ are derived from the velocity and are determined in accordance with the formulas:

$$\begin{aligned}
&w^{(x_s)}_{i,j,k,n}=\frac{V^{(x_s)}_{i+1,j,k,n}-V^{(x_s)}_{i-1,j,k,n}}{2h_{x_1}},\quad w2^{(x_s)}_{i,j,k,n}=\frac{V^{(x_s)}_{i,j+1,k,n}-V^{(x_s)}_{i,j-1,k,n}}{2h_{x_2}},\\
&w3^{(x_s)}_{i,j,k,n}=\frac{V^{(x_s)}_{i,j,k+1,n}-V^{(x_s)}_{i,j,k-1,n}}{2h_{x_3}}
\end{aligned} \tag{11}$$



(a) (b)

Figure 3. The configuration space of the initial and final particle distribution for the model of a sphere with a constant density.

Finding a solution is as follows. First, we set the initial distribution $D^{(x_s)}_{i,j,k,0}$ and $V^{(x_s)}_{i,j,k,0}$, where $\{i,j,k\}=\left\{0\le i\le N_{x_1}, 0\le j\le N_{x_2}, 0\le k\le N_{x_3}\right\}$. Next, using the formulas (10) and (11) we define $D^{(x_s)}_{i,j,k,1}$ and $V^{(x_s)}_{i,j,k,1}$ in the nodes of the mesh (9). Using the boundary conditions on the surface S or the conditions of symmetry of the problem, we find the missing values $D^{(x_s)}_{i,j,k,1}$ and $V^{(x_s)}_{i,j,k,1}$ in the nodes of the mesh $\{i,j,k\}=\left\{i=0,N_{x_1}, j=0,N_{x_2}, k=0,N_{x_3}\right\}$. Similarly, we find the value of $D^{(x_s)}_{i,j,k,n}$ and $V^{(x_s)}_{i,j,k,n}$ mesh functions on the next layers while $n>1$.

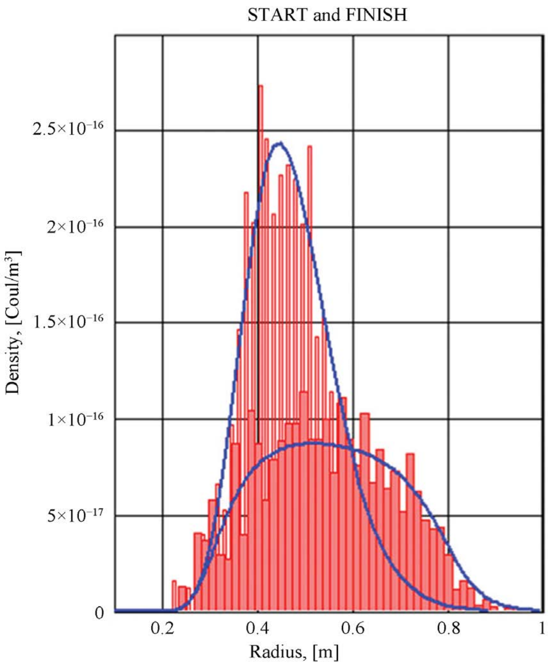
The difference schemes in Equations (10) and (11) can be applied to the functions with a smooth front. In the case of a discontinuous front another difference scheme adapted to this case must be used.

Figures 1(a) and **(b)** shows the initial and final charge density function distribution along the radius. The solid line shows the density function obtained by solving the problem (1) using the difference schemes in Equations (10) and (11). The bar chart shows the particle density to be calculated by PP (Particle-to-Particle) method. **Figure 4(a)** shows the function $\rho(r)$, and **Figure 4(b)** shows the function $\rho(r)r^2$. The area under the curve $\rho(r)r^2$ corresponds to the total charge of the system, which should remain constant.

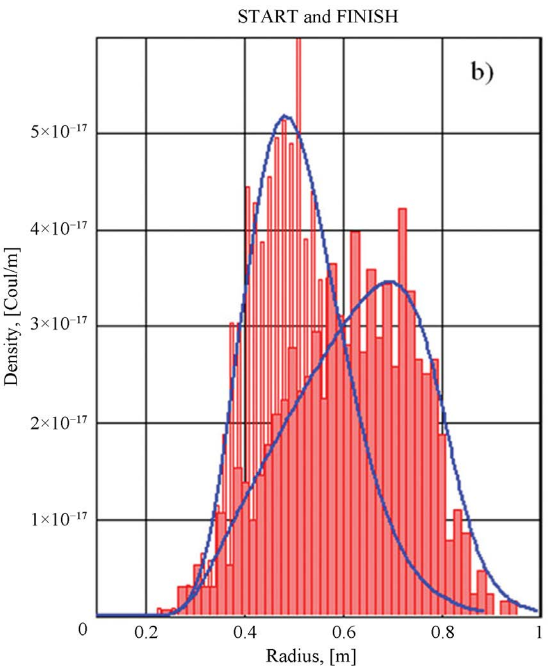
A comparison of the distributions in **Figure 4** shows that the Cauchy problem (1) and PP method have similar nature of the evolution of the charge density distribution function.

Figure 5 shows the evolution of the charge density distribution function at regular intervals for the Cauchy problem (1). We can see how the spreading of the spherical layer of the charge occurs.

Figure 6 shows the spatial distribution of the charge density distribution function at the initial and final time in the median plane.



(b)



(b)

Figure 4. **The initial and final distribution of the volume density of the particles for the model of the sphere with a normal logarithmic distribution of the charge density.**

4. Conclusion

In this paper, we considered the model solution of the Cauchy problem (1), with the zero initial velocity, and without external fields for the uniform and non-uniform distribution of the charge density. The results of the comparison of the calculations made by using the Particle-to-Particle (PP) method with calculations derived from the numerical solution of the Cauchy problem (1) are shown. The comparison showed a good agreement between the results. Thus, we tested the parameters of the Particle-to-Particle method, which is used in the real problems associated with the calculation of the space charge effect, for example, in accelerating installations. It is shown that there is a good correspondence to the theoretical data for the uniform case, for which there is an exact solution.

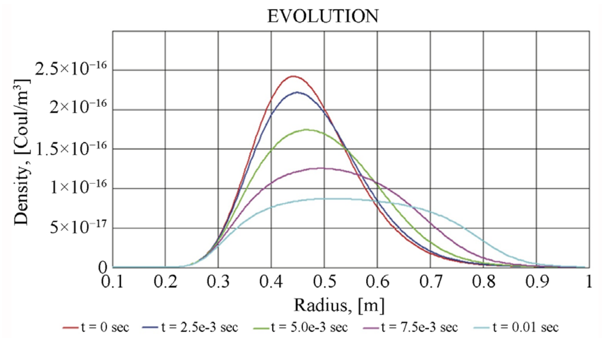
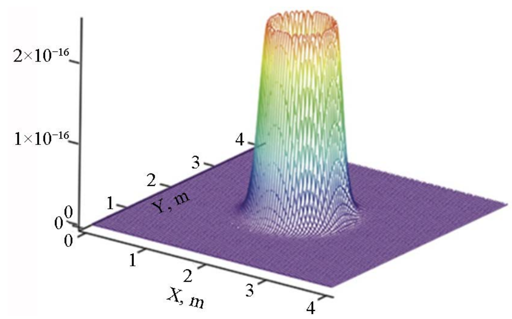
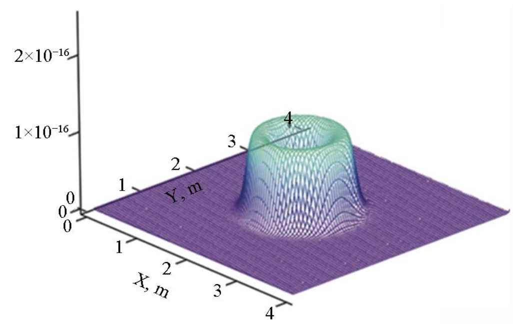


Figure 5. **The dependence of the distribution function of the charge density of the particles on time.**



(a)



(b)

Figure 6. **The initial and final charge density distribution in the median plane.**

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REFERENCES

[1] V. P. Maslov, "Equations of the Self-Consistent Field," *Itogi Nauki i Tekhniki*, *Sovremennye Problemy Matematiki*, Vol. 11, VINITI, Moscow, 1978, pp. 153-234.

[2] A. A. Vlasov, "Statistical Distribution Functions," Nauka, Moscow, 1968.

[3] N. G. Inozemtseva and B. I. Sadovnikov, "Evolution of Bogolyubov's Functional Hypothesis," *Physics of Particles and Nuclei*, Vol. 18, No. 4, 1987, p. 53.

[4] F. H. Harlow, "The Particle-in-Cell Method for Numerical Solution of Problems in Fluid Dynamics," *Proceedings of Symposium in Applied Mathematics*, Vol. 15, No. 10, 1963, p. 269.

[5] F. H. Harlow, S. S. Gryigoryan and Y. D. Shmyglevskiy, "The Particle-in-Cell Method for Numerical Solution of Problems in Hydrodynamics," Moscow, 1967, p. 383.