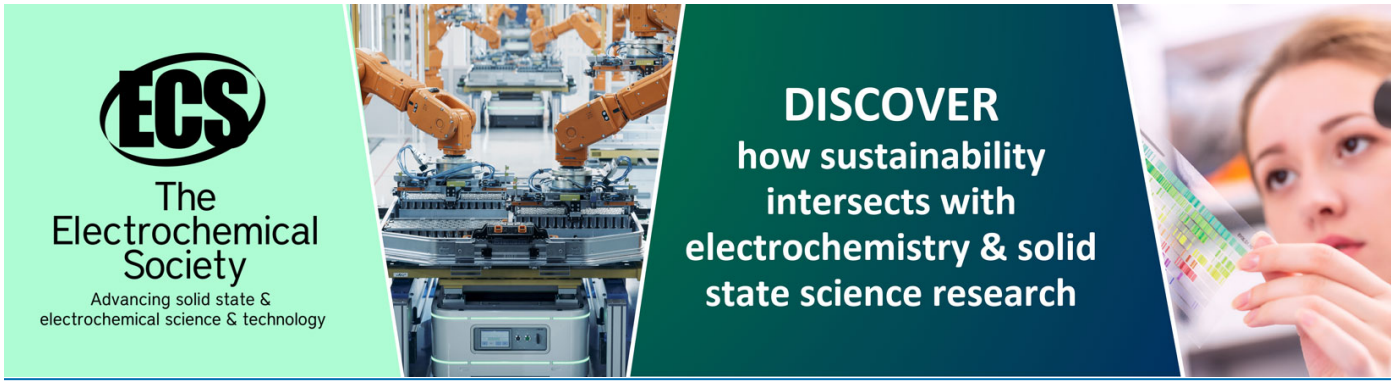
# Quantum shell effects in the hydrodynamic equations of a quantum fluid





IOP Conf. Series: Journal of Physics: Conf. Series **1238** (2019) 012037 doi:10.1088/1742-6596/1238/1/012037

# Quantum shell effects in the hydrodynamic equations of a quantum fluid.

**S E Kuratov[1], D S Shidlovski[1,2], I S Menshov[1,3] and S I Blinnikov[1,2]**

[1] Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya street 22, Moscow, 127055, Russia

[2] NRC "Kurchatov institute" – ITEP, Bol'shaya Cheremushkinskaya street 25, Moscow, 117218, Russia

[3] Keldysh Institute for Applied Mathematics Russian Academy Science

E-mail: ser.evg.kuratov@gmail.com, dmitry.shidlovski@yandex.ru

**Abstract.** Numerical analysis of the hydrostatic equilibrium of a compressed gas bubble was carried out by the DFT method. Based on this analysis, we modified the hydrodynamic equations of a quantum fluid taking into account quantum shell effects. An external force acting on the electronic subsystem is added to the modified hydrodynamic equations. A numerical algorithm for solving of the system of modified hydrodynamic equations is discussed.

Keywords: hydrodynamic equations, spatial distribution, hydrogen gas bubble, DFT method.

## 1. Introduction

The effect of the spatial heterogeneity of degenerate electron distribution in a spherical well was analyzed in [1]. The consequence of the effect is the appearance of an electric field acting on the ion system and causing its movement. The characteristic size of the inhomogeneity is of the order of the system size and, accordingly, by several orders of magnitude greater than the distance between the particles. So the relaxation of the ions can be described using the hydrodynamic approximation.

We analyze a spherical mesoscopic system – a compressed gas bubble of submicron size. The characteristic values of the thermodynamic quantities of the compressed gas are the following: $\rho_{gas} \sim$ (10-30) g/cm$^3$, $N_e \sim 10^{30-31}$ m$^{-3}$, $E_F \sim$ (20-100) eV, $T_i \sim T_e \sim$ (0.1-1) eV. All electrons are ionized and degenerated, and the ions are the classical gas.

The numerical analysis of the hydrostatic equilibrium of a gas bubble is presented in Section 2. Numerical simulation of the electron distribution was carried out by the DFT method. The analysis allowed us to formulate the simplest version of the hydrodynamic equations of a quantum liquid. The quantum shell effects are taken into account by introducing an external force (the oscillation potential) into the equation of motion of the degenerate electrons. Section 3 presents a numerical algorithm for solving the system of modified hydrodynamic equations. We applied this algorithm for the numerical analysis of ion relaxation in a compressed gas bubble.

## 2. Hydrostatic equilibrium of compressed gas bubble. DFT calculations.

To calculate distributions of electrons and ions in a spherically symmetrical bubble, we use DFT with spherical jellium background model and hydrostatic equation for ions [1, 2]. In the case

of a spherical symmetry the electron density and the density of ion liquid satisfy the system of equations (there we use atomic units, where $\hbar = c = e = 1$):

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_{\mathrm{KS}}(r) + \frac{l(l+1)}{2r^2}\right) P_{nl}(r) = \varepsilon_{nl} P_{nl}(r), \quad V_{\mathrm{KS}} = \varphi + V_{xc}, \tag{1}$$

$$n_e(r) = 2\sum_{n,l}(2l+1)\Theta_{nl}\frac{P_{nl}^2(r)}{4\pi r^2}, \tag{2}$$

$$-\frac{1}{n_{\mathrm{ion}}}\nabla P - Z_{\mathrm{ion}}\nabla\varphi = 0, \quad \text{with condition} \int_0^\infty 4\pi r^2 n_{\mathrm{ion}}\mathrm{d}r = N \tag{3}$$

$$\varphi(r) = \frac{1}{r}\int_0^r 4\pi s^2(n_{\mathrm{ion}}(s) - n_e(s))\mathrm{d}s + \int_r^{+\infty} 4\pi s(n_{\mathrm{ion}}(s) - n_e(s))\mathrm{d}s. \tag{4}$$

The first equation is the one-dimensional Kohn-Sham equation for radial wavefunctions $P_{nl}$, where $V_{xc}$ is the exchange-correlation potential in a local density approximation. Equation (3) is the hydrostatic equation for ion density $n_{\mathrm{ion}}$, where $P = n_{\mathrm{ion}}kT$. The last is the expression for the electric potential $\varphi$, which can be obtained from the Poisson equation. This system is solved self-consistently using simple iteration method. Equation (3) can be simply integrated

$$\ln(n_{\mathrm{ion}}) = -\frac{Z_{\mathrm{ion}}}{kT}\varphi - \ln T + C. \tag{5}$$

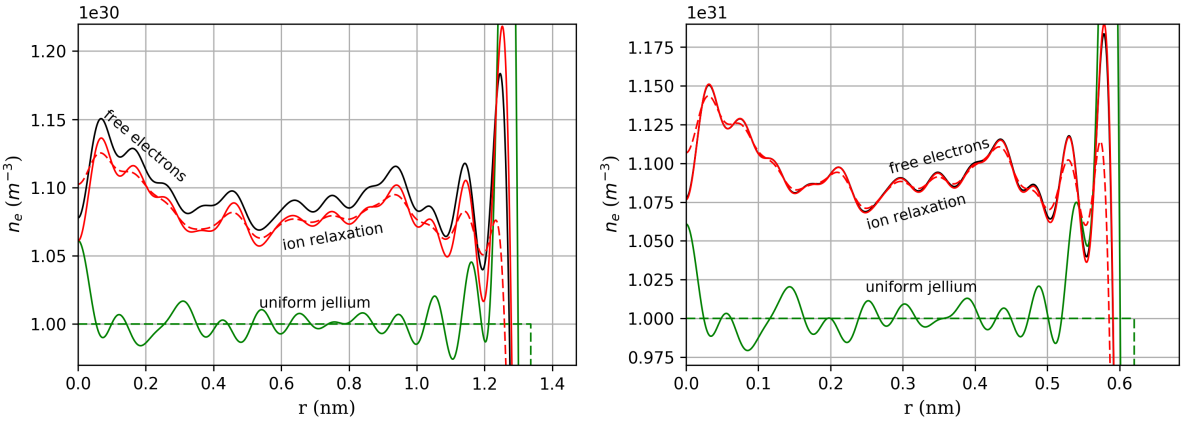



**Figure 1.** The density distributions of electrons (solid lines) and ions (dashed lines) for 10000 electrons at average density $10^{30}\mathrm{m}^{-3}$ (a) and $10^{31}\mathrm{m}^{-3}$ (b).

We have made several calculations for gas bubbles. Figure 1 shows the electron density distribution and the ion density in equilibrium for 10000 electrons at average density $10^{30}\mathrm{m}^{-3}$ and $10^{31}\mathrm{m}^{-3}$ with infinite potential wall at the border, the temperature of ions is $T_i = 10$ eV. There are also distributions of free electrons and electrons in the case of uniform ion jellium. It can be clearly seen that the density of ions is adjusted to the electron and the difference between density distributions is smaller for higher average density. At the same time the electron density get very close to free electron density and for average density $10^{31}\mathrm{m}^{-3}$ they are almost coincide.

Quantum mechanical calculations can be applied for a relatively small number of particles ($N < 10^5$), so we need to use simpler method such as quantum electron fluid model [3] for larger number of particles. We will consider equation for quantum electron fluid without

Bohm potential, but with osillation potential $U_{\rm osc}$, which should reproduce density distribution obtained in DFT calculations

$$-\frac{1}{\rho_e}\nabla p_e + \frac{e}{m_e}\nabla\varphi + \frac{e}{m_e}\nabla U_{\rm osc} = 0. \tag{6}$$

As we have seen earlier, the electron density in DFT calculations with ions in equilibrium and with an infinite potential border almost equal to the free electron density. Also $\nabla\varphi$ is rather small, because both densities are very close to each other. So the oscillation potential

$$e\nabla U_{\rm osc} \approx \frac{1}{n_e^{\rm free}}\nabla p_e(n_e^{\rm free}). \tag{7}$$

## 3. Numerical algorithm of hydrodynamic equations

We consider the sphere of the initial radius $R_0$ consisting of gas of degenerate electrons $n_e(r,t)$ and classical ions $n_i(r,t)$. It is assumed that the electron density satisfies the equilibrium condition at each time moment:

$$-e\frac{\partial}{\partial r}(\varphi + U_{\rm osc} - U_{\rm bar}) + \frac{1}{n_e}\frac{\partial p_e}{\partial r} = 0, \tag{8}$$

where $U_{\rm osc}$ and $U_{\rm bar}$ is the oscillation and barrier potentials:

$$U_{\rm bar} = -\frac{eV_0}{1+\exp[(R_0-r)/\delta]}, \quad U_{\rm osc} = C\left(\frac{\bar{n}}{10^{30}}^{1/3}\right)\frac{R_0(0)}{R_0(t)}f(r,R_0(t)) \tag{9}$$

where $\bar{n} = \bar{\rho}/m_i$ is the average electron density, and $V_0$ and $C$ are the characteristic amplitudes of the barrier and oscillation potentials, $\delta$ is the size of the barrier potential, and $f(r,R_0(t))$ the spatial profile of the oscillation potential.

The electron pressure depends on the local electron density and is determined by the following expression:

$$p_e = \frac{(3\pi^2)^{2/3}}{5}\frac{\hbar^2}{m_e}n_e^{5/3}. \tag{10}$$

The motion of the ion gas is a result of the action on the ions of the electrostatic field created by the instantaneous distribution of ions and electrons. The ion gas is assumed to be ideal, i.e., the effects of viscosity and thermal conductivity are negligible, and is calorically perfect with the equation of state $p = (\gamma-1)\rho\zeta$, where $\gamma = 5/3$ is the adiabatic exponent, $p$ is the pressure, $\zeta$ is the specific internal energy.

It can be shown that the influence of nonequilibrium between the distribution of ions and electrons takes place in a very small neighborhood of the wall. Therefore, in the gas dynamics calculations described below, it is assumed that there is a local equilibrium at all points inside the sphere $n_i = n_e$. Then the electron pressure will determine the ion distribution.

The medium inside the sphere is assumed to be electro neutral, therefore at each time moment the distributions of electrons and ions satisfy the condition of zero total charge:

$$\int_0^{R_0(t)} n_e(r,t)r^2dr = \int_0^{R_0(t)} n_i(r,t)r^2dr, \quad n_i = \rho/m_i, \tag{11}$$

where $m_i$ is the mass of ion.

The ion motion is described by the standard system of Euler equations for gas dynamics under the assumption of spherical symmetry, which is supplemented by the right-hand side

corresponding to the change in momentum and energy due to the electrostatic field produced by charged particles-gas ions and free electrons:

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial \rho U}{\partial r} = \dfrac{2}{r}\rho U, \\ \dfrac{\partial \rho U}{\partial t} + \dfrac{\partial \rho U^2 + p}{\partial r} = \dfrac{2}{r}\rho U^2 - \dfrac{e}{m_i}\rho\dfrac{\partial \varphi}{\partial r}, \\ \dfrac{\partial \rho E}{\partial t} + \dfrac{\partial \rho U H}{\partial r} = \dfrac{2}{r}\rho U H - \frac{e}{m_i}\rho U\dfrac{\partial \varphi}{\partial r}, \end{cases} \tag{12}$$

where $e$ is the electron charge, $E = U^2/2 + \zeta$ is the specific total ion energy, $H = \zeta + p/\rho$ is the specific total enthalpy, $\zeta = p/\rho(\gamma - 1)$ is the specific internal energy of the ions, $\gamma = 5/3$, $0 \le r \le R_0(t)$. The potential $\varphi$ is determined by the equation (8), where we use $n_i$ instead of $n_e$.

We write the system of equations (8), (12) in dimensionless form. To do this, we choose the scales of the characteristic physical quantities in the following form:

$\rho_* = 10^3 kg/m^3$ – density,
$L_* = 10^{-6} m$ – length,
$U_* = 10^3 m/s$,
$t_* = L_*/U_* = 10^{-9} s$,
$p_* = \rho_* U_*^2 = 10^9 N/m^2$ – preasure,
$\Theta_* = \dfrac{m_i U_*}{e t_*} \approx 1.875 * 10^4 V/m$ – electric field strength,
$\varphi_* = \dfrac{m_i U_*^2}{e} \approx 1.875 * 10^{-2} V$ – electric field potential.

The values of the physical parameters of the model:

$e = 1.6 * 10^{-19} C$ – electron charge,
$m_i = 3 * 10^{-27} kg$ – ion mass,
$\varepsilon_0 = 8.85 * 10^{-12} C/(V \cdot m)$ – dielectric constant of vacuum,
$\varepsilon = 10^4$ – relative dielectric constant of ions.

The system of equations (12) can be written in a conservative form. In dimensionless variables, it has the following form:

$$\begin{cases} \dfrac{\partial r^2 \rho}{\partial t} + \dfrac{\partial r^2 \rho U}{\partial r} = 0, \\ \dfrac{\partial r^2 \rho U}{\partial t} + \dfrac{\partial r^2 (\rho U^2 + p)}{\partial r} = 2rp - \rho r^2 \dfrac{\partial \varphi}{\partial r}, \\ \dfrac{\partial r^2 (\rho E)}{\partial t} + \dfrac{\partial r^2 (\rho U H)}{\partial r} = \rho U r^2 \dfrac{\partial \varphi}{\partial r}, \end{cases} \tag{13}$$

where the gradient of the potential

$$\frac{\partial \varphi}{\partial r} = K_1 \rho^{-1/3} \frac{\partial \rho}{\partial r} + K_3 \left[\frac{R_0(0)}{R_0(t)}\right]^2 \frac{\partial U_{\text{bar}}}{\partial r} - K_4 \frac{R_0(0)}{R_0(t)} \frac{\partial f(r, R_0(t))}{\partial r}. \tag{14}$$

Here $K_1$, $K_3$, $K_4$ are dimensionless constants:

$$K_1 = \frac{(3\pi^2)^{2/3}}{3} \frac{\hbar^2}{e m_e \varphi_*} n_*^{2/3}, \quad n_* = \rho_*/m_i,$$
$$K_3 = \frac{\hbar^2}{2 e m_e \varphi_*} \left(3\pi^2 \tfrac{\rho_0}{m_i}\right)^{2/3} \left[\frac{R_0(0)}{R_0(t)}\right]^2,$$
$$K_4 = C \frac{10^{-10} m}{\varphi_*} \left(\tfrac{\rho_0}{m_i}\right)^{1/3}.$$

If we introduce the total pressure $\pi = p + \frac{3}{5}K_1\rho^{5/3}$, the system of equations (13) can be rewritten as follows:

$$\begin{cases} \dfrac{\partial r^2\rho}{\partial t} + \dfrac{\partial r^2\rho U}{\partial r} = 0, \\ \dfrac{\partial r^2\rho U}{\partial t} + \dfrac{\partial r^2(\rho U^2+\pi)}{\partial r} - 2rp = -\rho r^2 \left\{ K_3 \left[\dfrac{R_0(0)}{R_0(t)}\right]^2 \dfrac{\partial U_{\text{bar}}}{\partial r} - K_4 \dfrac{R_0(0)}{R_0(t)} \dfrac{\partial f(r, R_0(t))}{\partial r} \right\}, \\ \dfrac{\partial r^2(\rho E)}{\partial t} + \dfrac{\partial r^2 U(E+\pi/\rho)}{\partial r} = \dfrac{3}{5}K_1\rho^{5/3}\dfrac{\partial r^2 u}{\partial r} - \\ \qquad\qquad -\rho r^2 \left\{ K_3 \left[\dfrac{R_0(0)}{R_0(t)}\right]^2 \dfrac{\partial U_{\text{bar}}}{\partial r} - K_4 \dfrac{R_0(0)}{R_0(t)} \dfrac{\partial f(r, R_0(t))}{\partial r} \right\}, \end{cases} \tag{15}$$

Except for the right-hand side, the system of equations (15) coincides exactly with the classical system of equations of gas dynamics. The EOS of the medium has the form

$$\pi = (\gamma - 1)\rho e + \frac{3}{5}K_1\rho^{5/3} \tag{16}$$

Therefore, the numerical integration (15) can be performed by the Godunov method [4]:

$$\mathbf{q}_i^{n+1} = \mathbf{q}_i^n - \frac{3\Delta t}{(r_{i+1/2}^{n+1})^3 - (r_{i-1/2}^{n+1})^3} \left[ (r_{i+1/2}^{n+1/2})^2 \mathbf{F}_{i+1/2} - (r_{i-1/2}^{n+1/2})^2 \mathbf{F}_{i-1/2} + \mathbf{S}_{\pi,i} + \mathbf{S}_{U,i} \right], \tag{17}$$

where

$$\mathbf{S}_{\pi,i} = \begin{bmatrix} 0 \\ \left( (r_{i+1/2}^{n+1})^2 - (r_{i-1/2}^{n+1})^2 \right) \pi_i \\ 0 \end{bmatrix}, \tag{18}$$

$$\mathbf{S}_{U,i} = \begin{bmatrix} 0 \\ \left( (r_{i+1/2}^{n+1})^3 - (r_{i-1/2}^{n+1})^3 \right) \rho_i S_{2,i} \\ \left( (r_{i+1/2}^{n+1})^2 U_{i+1/2} - (r_{i-1/2}^{n+1})^2 U_{i-1/2} \right) 3K_1\rho^{5/3} + \left( (r_{i+1/2}^{n+1})^3 - (r_{i-1/2}^{n+1})^3 \right) \rho_i U_i S_{3,i} \end{bmatrix},$$

Here, $S_{2,i}$ and $S_{3,i}$ the right-hand sides of the equations connected with the barrier and oscillation potential, and the values at the edges of the cells (half-integral indices) are determined from the solution of the Riemann problem. To solve the Riemann problem on the edges of countable cells, we use the local approximation of the EOS (16)

$$\pi = (\gamma - 1)\rho e + c_0^2(\rho - \rho_0) \tag{19}$$

where the parameters of the EOS $c_0$ and $\rho_0$ are approximated from the value of the local density by the following relations:

$$\rho_0 = \frac{2}{5}\rho, \quad c_0^2 = K_1\rho^{2/3}, \tag{20}$$

on the basis of splitting equations. At each time step, a hyperbolic system with zero right-hand side is first solved.

The Courant number is determined by the speed of sound of the system (13)

$$c^2 = \frac{\gamma(\pi + \pi_0)\rho e + \frac{3}{5}K_1\rho^{5/3}}{\rho}, \quad \pi_0 = \frac{2}{5\gamma}K_1\rho^{5/3}. \tag{21}$$

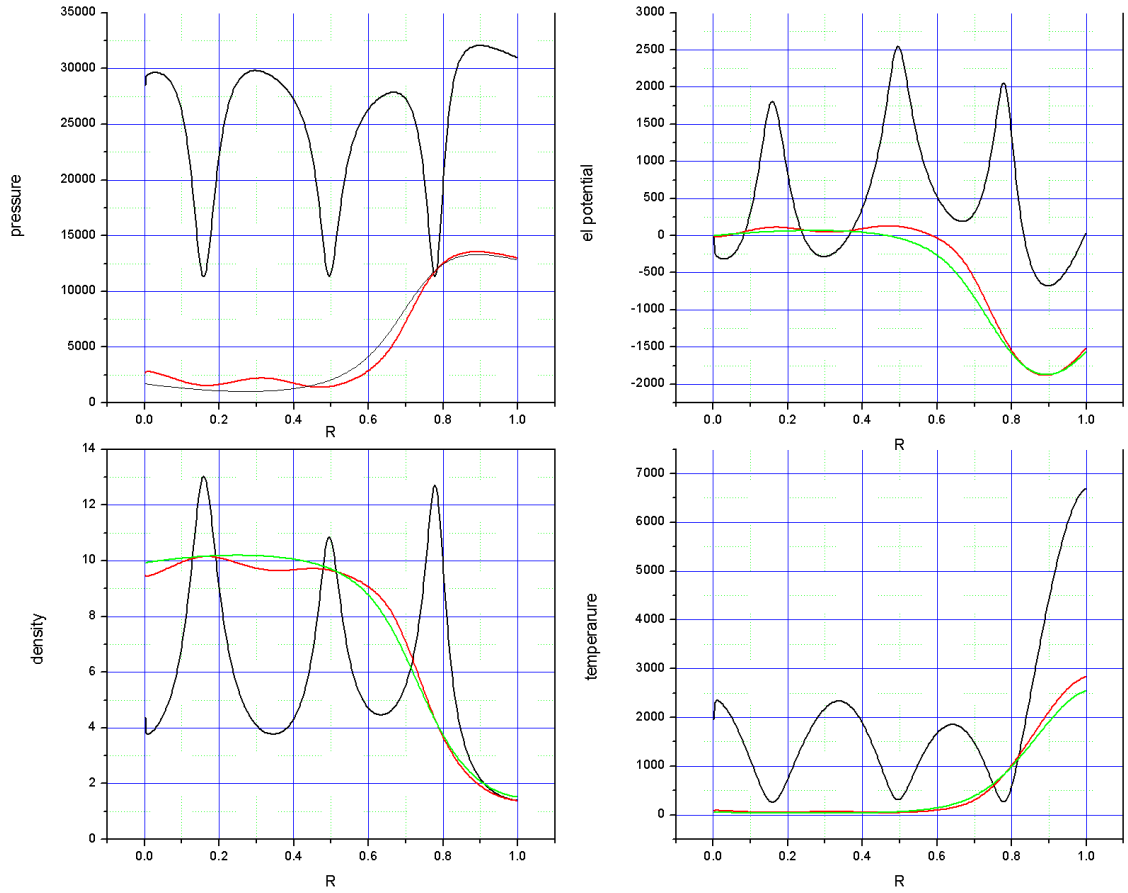



**Figure 2.** Stationary distributions of hydrodynamic quantities for different values of the oscillation potential amplitude.

The numerical scheme (17), (18) is used to solve the stationary problem of the distribution of the ion-electron system in a spherical region of radius 1 $\mu$m. The calculated grid consists of 300 equidistant cells. The number of Courant in the calculations was 0.5. Initial distributions in dimensionless quantities:

$$t = 0: \quad \rho = 5, \quad U = 0, \quad p = 21$$

Calculations were carried out with $\delta = 0.1R_0$ and three variants of the amplitude of the oscillation potential $C$ =10V, 1V, 0.1V. The results of the distributions of hydrodynamic quantities after the system's output to the stationary mode are shown in Fig. 2. Black color shows the results for $C = 10$V, red – $C = 1$V and green – $C = 0.1$V. We can see that the influence of the oscillation potential is significant for $C = 10$V and is insignificant for $C = 1$V and $C = 1$V.

## 4. Conclusion

Based on the analysis of the hydrostatic equilibrium of a compressed gas bubble, we derived modified hydrodynamic equations taking into account the quantum shell effects. The method is based on the addition of an oscillation potential to the equation of motion of the electrons. A numerical algorithm for solving a system of hydrodynamic equations based on the Godunov method is developed.

The results of numerical analysis of the relaxation of a compressed gas bubble are presented. They demonstrate the significant influence of the oscillation potential at hydrodynamic quantities of compressible gas bubble.

## References

[1] Kuratov S E, Shidlovski D S and Blinnikov S I 2018 *Journal of Physics: Conference Series* **1009** 012013
[2] Shidlovski D S and Mukhanov A E 2018 *Journal of Physics: Conference Series* **1009** 012012
[3] Shukla P K and Eliasson B 2010 (in Russian) *Uspekhi Fizicheskikh Nauk* **180**(1) 55–82
[4] Godunov S K, Zabrodin A V and Prokopov G P 1962 (in Russian) *USSR Computational Mathematics and Mathematical Physics* **1**(4) 1187