#### 1 **Application of Non-local Quantum Hydrodynamics to the Description** 2 of the Charged Density Waves in the Graphene Crystal Lattice. 3 4 5 Boris V. Alexeev, Irina V. Ovchinnikova 6 Moscow Lomonosov University of Fine Chemical Technologies (MITHT) 7 Prospekt Vernadskogo, 86, Moscow 119570, Russia 8 Boris.Vlad.Alexeev@gmail.com 9 e-mail: boris.vlad.alexeev@gmail.com 10 11 The motion of the charged particles in graphene in the frame of the quantum non-local hydrodynamic description is considered. It is shown as results of the mathematical modeling that 12 13 the mentioned motion is realizing in the soliton forms. The dependence of the size and structure of 14 solitons on the different physical parameters is investigated. 15 Key words: Foundations of the theory of transport processes; The theory of solitons; 16 17 Generalized hydrodynamic equations; High temperature superconductivity; Quantum non-local 18 hydrodynamics, Theory of transport processes in graphene. 19 PACS: 67.55.Fa, 67.55.Hc 20 1. Introduction. Preliminary remarks. 21 22 23 The possibility of the non local physics application in the theory of superconductivity is 24 investigated in [1-3]. It is shown that by the superconducting conditions the relay ("estafette") 25 motion of the soliton' system ("lattice ion – electron") is realizing by the absence of chemical 26 bonds. From the position of the quantum hydrodynamics the problem of creation of the high 27 temperature superconductors leads to finding of materials which lattices could realize the soliton' 28 motion without destruction. These materials should be created using the technology of quantum 29 dots. 30 Non-local physics demonstrates its high efficiency in many fields – from the atom structure 31 problems to cosmology [4 - 16]. Mentioned works contain not only strict theory, but also delivering 32 the qualitative aspects of theory without excessively cumbersome formulas. As it is shown (see, for 33 example [4,5,7 - 11]) the theory of transport processes (including quantum mechanics) can be 34 considered in the frame of unified theory based on the non-local physical description.

This paper is directed on investigation of possible applications of the non-local quantum hydrodynamics in the theory of transport processes in graphene including the effects of the charge density waves (CDW). Is known that graphene, a single-atom-thick sheet of graphite, is a new material which combines aspects of semiconductors and metals. For example the mobility, a measure of how well a material conducts electricity, is higher than for other known material at room temperature. In graphene, a resistivity is of about 1.0 microOhm-cm (resistivity defined as a specific measure of resistance; the resistance of a piece material is its resistivity times its length and divided by its cross-sectional area). This is about 35 percent less than the resistivity of copper, the lowest resistivity material known at room temperature.

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Measurements lead to conclusion that the influence of thermal vibrations on the conduction of electrons in graphene is extraordinarily small. From the other side the typical reasoning exists:

46 "In any material, the energy associated with the temperature of the material causes the atoms 47 of the material to vibrate in place. As electrons travel through the material, they can bounce off 48 these vibrating atoms, giving rise to electrical resistance. This electrical resistance is "intrinsic" to 49 the material: it cannot be eliminated unless the material is cooled to absolute zero temperature, and 50 hence sets the upper limit to how well a material can conduct electricity."

51 Obviously this point of view leads to the principal elimination of effects of the high 52 temperature superconductivity. From the mentioned point of view the restrictions in mobilities of 53 known semiconductors can be explained as the influence of the thermal vibration of the atoms. The limit to mobility of electrons in graphene is about 200,000  $cm^2/(V \cdot s)$ ) at room temperature, 54 compared to about 1,400  $cm^2/(V \cdot s)$  in silicon, and 77,000  $cm^2/(V \cdot s)$  in indium antimonide, the 55 56 highest mobility conventional semiconductor known. The opinion of a part of investigators can be 57 formulated as follows: "Other extrinsic sources in today's fairly dirty graphene samples add some 58 extra resistivity to graphene," (see for example [17]) "so the overall resistivity isn't quite as low as 59 copper's at room temperature yet. However, graphene has far fewer electrons than copper, so in 60 graphene the electrical current is carried by only a few electrons moving much faster than the 61 electrons in copper." Mobility determines the speed at which an electronic device (for instance, a 62 field-effect transistor, which forms the basis of modern computer chips) can turn on and off. The 63 very high mobility makes graphene promising for applications in which transistors much switch 64 extremely fast, such as in processing extremely high frequency signals. The low resistivity and 65 extremely thin nature of graphene also promises applications in thin, mechanically tough, electrically conducting, transparent films. Such films are sorely needed in a variety of electronics 66 67 applications from touch screens to photovoltaic cells.

In the last years the direct observation of the atomic structures of superconducting materials (as usual superconducting materials in the cuprate family like YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.67</sub> ( $T_c = 67$  K)) was realized with the scanning tunneling microscope (STM) and other instruments, STMs scan a surface in steps smaller than an atom. 72 Superconductivity, in which an electric current flows with zero resistance, was first 73 discovered in metals cooled very close to absolute zero. New materials called cuprates - copper 74 oxides "doped" with other atoms -- superconduct as "high" as minus 123 Celsius. Some conclusions 75 from direct observations [18, 19]:

- 76 1. Observations of high-temperature superconductors show an "energy gap" where 77 electronic states are missing. Sometimes this energy gap appears but the material 78 still does not superconduct -- a so-called "pseudogap" phase. The pseudogap 79 appears at higher temperatures than any superconductivity, offering the promise 80 of someday developing materials that would superconduct at or near room 81 temperature.
- 82 2. STM image of a partially doped cuprate superconductor shows regions with an 83 electronic "pseudogap". As doping increases, pseudogap regions spread and 84 connect, making the whole sample a superconductor.
- 85 3. High temperature superconductivity in layered cuprates can develop from an electronically ordered state called a charge density wave (CDW). The results of 86 87 observation can be interpreted as the creation of the "checkerboard pattern" due 88 to the modulation of the atomic positions in the CuO<sub>2</sub> layers of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6+x</sub> 89 caused by the charge density wave.
- 90 4. Application of the method of high-energy X-ray diffraction shows that a CDW 91 develops at zero field in the normal state of superconducting YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.67</sub> 92  $(T_c = 67 \text{ K})$ . Below  $T_c$  the application of a magnetic field suppresses 93 superconductivity and enhances the CDW. It means that the high- $T_{\rm c}$ 94 superconductivity forms from a pre-existing CDW environment.

95 Important conclusion: high temperature superconductors demonstrate new type of electronic order 96 and modulation of atomic positions. As it was shown in [1,3] the delivered above graphene 97 properties can be explained only in the frame of the self-consistent non-local quantum theory (see 98 for example [4,5]) which leads to appearance of the soliton waves moving in graphene.

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- 100

### 2. Generalized quantum hydrodynamic equations describing the soliton movement in 101 the crystal lattice.

102

103 Let us consider the charge density waves which are periodic modulation of conduction 104 electron density. From direct observations of charge density waves follow that CDW develop at 105 zero external fields. For our aims is sufficient in the following to suppose that the effective charge 106 movement was created in grapheme lattice as result of an initial fluctuation.

107 The movement of the soliton waves at the presence of the external electrical potential108 difference will be considered also in this article.

109 This effective charge is created due to interference of the induced electron waves and 110 correlating potentials as result of the polarized modulation of atomic positions. Therefore in this 111 approach the conduction in grapheme convoys the transfer of the positive  $(+e, m_n)$  and negative (-112  $e, m_e$ ) charges. Let us formulate the problem in detail. The non-stationary 1D motion of the combined soliton is considered under influence of the self-consistent electric forces of the potential 113 114 and non-potential origin. It was shown [1, 3] that mentioned soliton can exists without a chemical bond formation. For better understanding of the situation let us investigate the situation for the case 115 when the external forces are absent. Introduce the coordinate system ( $\xi = x - Ct$ ) moving along the 116 positive direction of the x axis with the velocity  $C = u_0$ , which is equal to the phase velocity of 117 118 this quantum object.

119 Let us find the soliton type solutions for the system of the generalized quantum equations for 120 two species mixture [1, 3, 5, 11]. The graphene crystal lattice is 2D flat structure which is 121 considered in the moving coordinate system ( $\xi = x - u_0 t$ , y).

- Write down the system of equations [1, 3, 5, 11] for the two component mixture of charged particles without taking into account the component's internal energy in the dimensionless form, where dimensionless symbols are marked by tildes. We begin with introduction the scales:
- 125  $u = u_0 \tilde{u}$  hydrodynamic velocity;

126 
$$\xi = x_0 \tilde{\xi}$$
,  $y = x_0 \tilde{y}$ 

- 127  $\varphi = \varphi_0 \tilde{\varphi}$  self-consistent electric potential;
- 128  $\rho_e = \rho_0 \tilde{\rho}_e$ ,  $\rho_p = \rho_0 \tilde{\rho}_p$  densities for the electron and positive species;
- 129  $p_e = \rho_0 V_{0e}^2 \tilde{p}_e, \ p_p = \rho_0 V_{0p}^2 \tilde{p}_p$  quantum electron pressure and the pressure of positive species,
- 130 where  $V_{0e}$ ,  $V_{0p}$  the scales for thermal velocities for the electron and positive species;
- 131  $F_e = \frac{e\varphi_0}{m_e x_0} \tilde{F}_e$ ,  $F_p = \frac{e\varphi_0}{m_p x_0} \tilde{F}_p$  the forces acting on the mass unit of electrons and the positive
- 132 particles, where  $m_e$ ,  $m_p$  are masses of electrons and the positive particles.
- 133 Non-local parameters can be written in the form (see also [1, 3, 10, 11])

134 
$$\tau_{e} = \frac{x_{0}H}{u_{0}\tilde{u}^{2}}, \ \tau_{p} = \frac{m_{e}x_{0}H}{m_{p}u_{0}\tilde{u}^{2}}, \ \frac{1}{\tau_{ep}} = \frac{1}{\tau_{e}} + \frac{1}{\tau_{p}} = \frac{u_{0}}{x_{0}}\frac{\tilde{u}^{2}}{H}\left(1 + \frac{m_{p}}{m_{e}}\right).$$
(1)

135 Dimensionless parameter  $H = \frac{N_R \hbar}{m_e x_0 u_0}$  is introduced,  $N_R$  - entire number. Let us introduce also the

136 following dimensionless parameters

137 
$$R = \frac{e\rho_0 x_0^2}{m_e \varphi_0}, \ E = \frac{e\varphi_0}{m_e u_0^2}.$$
 (2)

- Taking into account the introduced values the following system of dimensionless non-local
- hydrodynamic equations for the 2D soliton description can be written (see also [1 5]):
- Dimensionless Poisson equation for the self-consistent electric field:

142 
$$\frac{\partial^{2} \tilde{\varphi}}{\partial \tilde{\xi}^{2}} + \frac{\partial^{2} \tilde{\varphi}}{\partial \tilde{y}^{2}} = -4\pi R \left\{ \frac{m_{e}}{m_{p}} \left[ \tilde{\rho}_{p} - \frac{m_{e}H}{m_{p}\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left( \tilde{\rho}_{p} \left( \tilde{u} - 1 \right) \right) \right] - \left[ \tilde{\rho}_{e} - \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left( \tilde{\rho}_{e} \left( \tilde{u} - 1 \right) \right) \right] \right\}.$$
143 (3)

Continuity equation for the positive particles: 

$$\frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{p} (1 - \tilde{u}) \right] + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{p} (\tilde{u} - 1)^{2} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} E \tilde{\rho}_{p} \tilde{F}_{p\xi} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} E \tilde{\rho}_{p} \tilde{F}_{p\xi} \right] \right\} = 0$$

$$(4)$$
147 Continuity equation for electrons:

- Continuity equation for electrons:

$$\frac{\partial}{\partial \tilde{\xi}} [\tilde{\rho}_{e}(1-\tilde{u})] + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} [\tilde{\rho}_{e}(\tilde{u}-1)^{2}] \right\} + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{e} - \tilde{\rho}_{e} E \tilde{F}_{e\xi} \right] \right\} + \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{y}} \tilde{p}_{e} - \tilde{\rho}_{e} E \tilde{F}_{ey} \right] \right\} = 0$$
(5)

Momentum equation for the *x* direction:

$$\frac{\partial}{\partial \xi} \left\{ \left( \widetilde{\rho}_{p} + \widetilde{\rho}_{e} \right) \widetilde{u} \left( \widetilde{u} - 1 \right) + \frac{V_{0p}^{2}}{u_{0}^{2}} \widetilde{p}_{p} + \frac{V_{0e}^{2}}{u_{0}^{2}} \widetilde{p}_{e} \right\} - \frac{m_{e}}{m_{p}} \widetilde{\rho}_{p} E \widetilde{F}_{p\xi} - \widetilde{\rho}_{e} E \widetilde{F}_{e\xi} + \\
+ \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\widetilde{u}^{2}} \left[ \frac{\partial}{\partial \xi} \left( 2 \frac{V_{0p}^{2}}{u_{0}^{2}} \widetilde{p}_{p} (1 - \widetilde{u}) - \widetilde{\rho}_{p} \widetilde{u} (1 - \widetilde{u})^{2} \right) - \frac{m_{e}}{m_{p}} \widetilde{\rho}_{p} E \widetilde{F}_{p\xi} (1 - \widetilde{u}) \right] \right\} + \\
+ \frac{\partial}{\partial \xi} \left\{ \frac{H}{\widetilde{u}^{2}} \left[ \frac{\partial}{\partial \xi} \left( 2 \frac{V_{0e}^{2}}{u_{0}^{2}} \widetilde{p}_{e} (1 - \widetilde{u}) - \widetilde{\rho}_{e} \widetilde{u} (1 - \widetilde{u})^{2} \right) - \widetilde{\rho}_{e} E \widetilde{F}_{e\xi} (1 - \widetilde{u}) \right] \right\} + \\
+ \frac{H}{\widetilde{u}^{2}} E \left( \frac{m_{e}}{m_{p}} \right)^{2} \widetilde{F}_{p\xi} \left( \frac{\partial}{\partial \xi} \left( \widetilde{\rho}_{p} (\widetilde{u} - 1) \right) \right) + \frac{H}{\widetilde{u}^{2}} E \widetilde{F}_{e\xi} \left( \frac{\partial}{\partial \xi} \left( \widetilde{\rho}_{e} (\widetilde{u} - 1) \right) \right) - \\
153 - \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\widetilde{u}^{2}} \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \left( \widetilde{p}_{p} \widetilde{u} \right) \right\} - \frac{\partial}{\partial \xi} \left\{ \frac{H}{\widetilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \left( \widetilde{p}_{e} \widetilde{u} \right) \right\} -$$

$$154 \qquad -\frac{m_{e}}{m_{p}}\frac{\partial}{\partial\widetilde{y}}\left\{\frac{H}{\widetilde{u}^{2}}\frac{V_{0p}^{2}}{u_{0}^{2}}\frac{\partial}{\partial\widetilde{y}}\left(\widetilde{p}_{p}\widetilde{u}\right)\right\}-\frac{\partial}{\partial\widetilde{y}}\left\{\frac{H}{\widetilde{u}^{2}}\frac{V_{0e}^{2}}{u_{0}^{2}}\frac{\partial}{\partial\widetilde{y}}\left(\widetilde{p}_{e}\widetilde{u}\right)\right\}+$$
$$155 \qquad +\left(\frac{m_{e}}{m_{p}}\right)^{2}\frac{\partial}{\partial\widetilde{\xi}}\left\{\frac{H}{\widetilde{u}^{2}}E\left[\widetilde{F}_{p\xi}\widetilde{\rho}_{p}\widetilde{u}\right]\right\}+\frac{\partial}{\partial\widetilde{\xi}}\left\{\frac{H}{\widetilde{u}^{2}}E\left[\widetilde{F}_{e\xi}\widetilde{\rho}_{e}\widetilde{u}\right]\right\}+$$

156 
$$+\left(\frac{m_e}{m_p}\right)^2 \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{py} \tilde{\rho}_p \tilde{u}] \right\} + \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{ey} \tilde{\rho}_e \tilde{u}] \right\} = 0$$

Energy equation for the positive particles: 

$$\frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{p} \tilde{u}^{2} (\tilde{u}-1) + 5 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u} - 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \right] - 2 \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \tilde{F}_{p\xi} \tilde{u} + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{m_{e}}{m_{p}} \left[ \frac{\partial}{\partial \tilde{\xi}} \left( -\tilde{\rho}_{p} \tilde{u}^{2} (1-\tilde{u})^{2} + 7 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u} (1-\tilde{u}) + 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} (\tilde{u}-1) - \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u}^{2} - 5 \frac{V_{0p}^{4}}{u_{0}^{4}} \frac{\tilde{\rho}_{p}^{2}}{\tilde{\rho}_{p}} \right] - 2 \frac{m_{e}}{m_{p}} E \tilde{F}_{p\xi} \tilde{\rho}_{p} \tilde{u} (1-\tilde{u}) + 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} (\tilde{u}-1) - \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u}^{2} - 5 \frac{V_{0p}^{4}}{u_{0}^{4}} \frac{\tilde{\rho}_{p}^{2}}{\tilde{\rho}_{p}} \right] - 2 \frac{m_{e}}{m_{p}} E \tilde{F}_{p\xi} \tilde{\rho}_{p} \tilde{u} (1-\tilde{u}) + \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} \tilde{u}^{2} E \tilde{F}_{p\xi} + 5 \frac{m_{e}}{m_{p}} \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} E \tilde{F}_{p\xi} \right]$$

$$159 \qquad -\frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{m_{e}}{m_{p}} \left[ \frac{\partial}{\partial \tilde{y}} \left( \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u}^{2} + 5 \frac{V_{0p}^{4}}{u_{0}^{4}} \frac{\tilde{p}_{p}^{2}}{\tilde{\rho}_{p}} \right) - \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \tilde{F}_{py} \tilde{u}^{2} - 5 \frac{m_{e}}{m_{p}} \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} E \tilde{F}_{py} \right] \right\} - 2\frac{H}{\tilde{u}^{2}} \left( \frac{m_{e}}{m_{p}} \right)^{3} \tilde{\rho}_{p} E^{2} \left[ \left( \tilde{F}_{p\xi} \right)^{2} + \left( \tilde{F}_{py} \right)^{2} \right] + 2\frac{H}{\tilde{u}^{2}} \left( \frac{m_{e}}{m_{p}} \right)^{2} E \tilde{F}_{p\xi} \left[ \frac{\partial}{\partial \tilde{\xi}} \left( \tilde{\rho}_{p} \tilde{u} (1 - \tilde{u}) \right) \right] - 2\frac{H}{\tilde{u}^{2}} \left( \frac{m_{e}}{m_{p}} \right)^{3} \tilde{\rho}_{p} E^{2} \left[ \left( \tilde{F}_{p\xi} \right)^{2} + \left( \tilde{F}_{py} \right)^{2} \right] + 2\frac{H}{\tilde{u}^{2}} \left( \frac{m_{e}}{m_{p}} \right)^{2} E \tilde{F}_{py} \left[ \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{y}} \tilde{\rho}_{p} \right] = -\frac{\tilde{u}^{2}}{Hu_{0}^{2}} \left( V_{0p}^{2} \tilde{\rho}_{p} - \tilde{\rho}_{e} V_{0e}^{2} \right) \left( 1 + \frac{m_{p}}{m_{e}} \right)$$

$$160$$

$$161 \qquad (7)$$

$$\begin{array}{ll} 161 \\ 162$$

(8)

(6)

165 The right hand sides of the energy equations are written in the relaxation forms following from166 BGK kinetic approximation.

167 Acting forces are the sum of three terms: the self-consistent potential force (scalar potential 168  $\varphi$ ), connected with the displacement of positive and negative charges, potential forces originated 169 by the grapheme crystal lattice (potential U) and the external electrical field creating the intensity 170 E. As result the following dimensionless relations are valid

171 
$$\widetilde{\mathbf{F}}_{\mathbf{p}\xi} = -\frac{\partial \widetilde{\boldsymbol{\varphi}}}{\partial \widetilde{\boldsymbol{\xi}}} - \frac{\partial \widetilde{\boldsymbol{U}}}{\partial \widetilde{\boldsymbol{\xi}}} + \widetilde{\boldsymbol{E}}_{\boldsymbol{\xi}}, \quad \widetilde{\mathbf{F}}_{\mathbf{e}\xi} = \frac{\partial \widetilde{\boldsymbol{\varphi}}}{\partial \widetilde{\boldsymbol{\xi}}} + \frac{\partial \widetilde{\boldsymbol{U}}}{\partial \widetilde{\boldsymbol{\xi}}} - \widetilde{\boldsymbol{E}}_{\boldsymbol{\xi}},$$

172 
$$\widetilde{F}_{py} = -\frac{\partial \widetilde{\varphi}}{\partial \widetilde{y}} - \frac{\partial \widetilde{U}}{\partial \widetilde{y}} + \widetilde{E}_{y}, \qquad \widetilde{F}_{ey} = \frac{\partial \widetilde{\varphi}}{\partial \widetilde{y}} + \frac{\partial \widetilde{U}}{\partial \widetilde{y}} - \widetilde{E}_{y}.$$
(9)

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182

174 Graphene is a single layer of carbon atoms densely packed in a honeycomb lattice. Figure 1 reflects

175 the structure of grapheme as the 2D hexagonal carbon crystal, the distance *a* between the nearest 176 atoms is equal to  $a = 0.142 \ nm$ .



x

180 Elementary cell contains two atoms (for example A and B, Fig. 1) and the primitive lattice

181 vectors are given by

$$\mathbf{a}_1 = \frac{a}{2}(3;\sqrt{3}), \ \mathbf{a}_2 = \frac{a}{2}(3;-\sqrt{3}).$$

183 Coordinates of the nearest atoms to the given atom define by vectors

184 
$$\boldsymbol{\delta}_1 = \frac{a}{2} (1; \sqrt{3}), \ \boldsymbol{\delta}_2 = \frac{a}{2} (1; -\sqrt{3}), \ \boldsymbol{\delta}_3 = -a(1;0).$$

185 Six neighboring atoms of the second order are placed in knots defined by vectors

186  $\boldsymbol{\delta}_1' = \pm \mathbf{a}_1, \ \boldsymbol{\delta}_2' = \pm \mathbf{a}_2, \ \boldsymbol{\delta}_3' = \pm (\mathbf{a}_2 - \mathbf{a}_1).$ 

Let us take the first atom of the elementary cell in the origin of the coordinate system (Fig.

(12)

(14)

1) and compose the radii-vector of the second atom with respect to the basis  $\mathbf{a}_1 \ \mbox{i} \ \mathbf{a}_2$ : 188  $\mathbf{r}_1 = u\mathbf{a}_1 + v\mathbf{a}_2 = u\left(3\frac{a}{2}\mathbf{e}_x + \sqrt{3}\frac{a}{2}\mathbf{e}_y\right) + v\left(3\frac{a}{2}\mathbf{e}_x - \sqrt{3}\frac{a}{2}\mathbf{e}_y\right).$ 189 (10)

190 Let us find *u* u *v*, taking into account that

191 
$$\mathbf{r}_{1} = \mathbf{\delta}_{1} = \frac{a}{2} \left( \mathbf{l}; \sqrt{3} \right) = \frac{a}{2} \mathbf{e}_{x} + \frac{a}{2} \sqrt{3} \mathbf{e}_{y} \,. \tag{11}$$

Equalizing (10)  $\mu$  (11), we have  $u = \frac{2}{3}$ ,  $v = -\frac{1}{3}$ , then 192

193 
$$\mathbf{r}_1 = \frac{2}{3} \mathbf{a}_1 - \frac{1}{3} \mathbf{a}_2.$$

Assume that  $V_1(\mathbf{r})$  is the periodical potential created by one sublattice. Then potential of 194 195 crystal is

196 
$$V(\mathbf{r}) = V_1(\mathbf{r}) + V_1(\mathbf{r} - \mathbf{r}_1) = \sum_{n=0}^{1} V_1(\mathbf{r} - \mathbf{r}_n).$$
(13)

197 Atoms in crystal form the periodic structure and as the consequence the corresponding potential is 198 periodic function

- $V_1(\mathbf{r}) = V_1(\mathbf{r} + \mathbf{a}_m),$  $\mathbf{a}_m = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2,$ 199
- 200 where for 2D structure
- 201

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and  $m_1 \bowtie m_2$  are arbitrary entire numbers. Expanding  $V_1(\mathbf{r})$  in the Fourier series one obtains 202

203

204 In our case the both basis atoms (n=0,1) are the same. Here

$$\mathbf{b} = g_1 \mathbf{b}_1 + g_2 \mathbf{b}_2$$

 $\mathbf{b}_1 \ \mathbf{u} \ \mathbf{b}_2$  are the translational vectors of the reciprocal lattice. For graphene 206

207 
$$\mathbf{b}_1 = \frac{2\pi}{3a} (1; \sqrt{3}), \quad \mathbf{b}_2 = \frac{2\pi}{3a} (1; -\sqrt{3}).$$
 (15)

 $V_1(\mathbf{r}-\mathbf{r}_n) = \sum_{\mathbf{b}} V_{\mathbf{b}} e^{i\mathbf{b}\cdot(\mathbf{r}-\mathbf{r}_n)}$ .

208 Then 🔪

209 
$$V(\mathbf{r}) = \sum_{\mathbf{b}} \sum_{n=0}^{1} V_{1\mathbf{b}} e^{i\mathbf{b}\cdot(\mathbf{r}-\mathbf{r}_n)} = \sum_{\mathbf{b}} V_{\mathbf{b}} e^{i\mathbf{b}\cdot\mathbf{r}} , \qquad (16)$$

where  $V_{\mathbf{b}} = V_{\mathbf{lb}} \cdot \sum_{n} e^{-i\mathbf{b}\cdot\mathbf{r}_{n}} = V_{\mathbf{lb}} \cdot S_{\mathbf{b}}$ . The structure factor  $S_{\mathbf{b}}$  for graphene: 210

211 
$$S_{\mathbf{b}} = e^{-i\mathbf{b}\cdot\mathbf{0}} + e^{-i\mathbf{b}\cdot\left(\frac{2}{3}\mathbf{a}_{1}-\frac{1}{3}\mathbf{a}_{2}\right)} = 1 + e^{i\frac{2\pi}{3}(g_{2}-2g_{1})}.$$
 (17)

213 
$$V(\mathbf{r}) = \sum_{g_1, g_2} V_{1g_1, g_2} e^{i(g_1\mathbf{b}_1 + g_2\mathbf{b}_2)\mathbf{r}} \left(1 + e^{i\frac{2\pi}{3}(g_2 - 2g_1)}\right).$$
(18)

For the approximate calculation we use the terms of the series with  $|g_1| \le 2$ ,  $|g_2| \le 2$ . Therefore 214

$$V(\mathbf{r}) = 2V_{1,(00)} + 4V_{1,(10)} \left( \cos\left(\frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}\right) \cos\left(\frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}\right) + \cos\left(\frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r} + \frac{2\pi}{3}\right) \cos\left(\frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}\right) \right) + 4V_{1,(10)} \left( \cos\left(\frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}\right) + \cos\left(\frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}\right) \right) + \frac{2\pi}{3} \cos\left(\frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}\right) + \frac{2\pi}{3} \cos\left(\frac{1}{3}(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}\right) + \frac{2\pi}{3} \cos\left(\frac{1$$

216 
$$+2V_{1,(11)}\left(\cos((\mathbf{b}_{1}+\mathbf{b}_{2})\cdot\mathbf{r})+\cos\left((\mathbf{b}_{1}+\mathbf{b}_{2})\cdot\mathbf{r}-\frac{2\pi}{3}\right)+2\cos((\mathbf{b}_{1}-\mathbf{b}_{2})\cdot\mathbf{r})\right)$$

217 
$$-4V_{1,(20)}\cos((\mathbf{b}_2-\mathbf{b}_1)\cdot\mathbf{r})\cos((\mathbf{b}_2+\mathbf{b}_1)\cdot\mathbf{r}+\frac{2\pi}{3})+$$

218 + 
$$2V_{1,(12)}\left(2\cos((\mathbf{b}_1+2\mathbf{b}_2)\cdot\mathbf{r})+2\cos((2\mathbf{b}_1+\mathbf{b}_2)\cdot\mathbf{r})+\right)$$

219 + 
$$\cos\left((\mathbf{b}_1 - 2\mathbf{b}_2) \cdot \mathbf{r} - \frac{\pi}{3}\right) - \cos\left((2\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r} - \frac{2\pi}{3}\right)\right) +$$

220 + 
$$2V_{1,(22)}\left(2\cos(2(\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r}) - \cos\left(2(\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r} - \frac{2\pi}{3}\right)\right).$$
 (19)

Using the vectors  $\mathbf{b}_1$  and  $\mathbf{b}_2$  of the reciprocal lattice from (15) and coordinates x and y one obtains 221 222 from (19):

223 
$$V(x, y) = 2V_{1,(00)} + 4V_{1,(10)}\cos\left(\frac{2\pi}{3a}x + \frac{\pi}{3}\right)\cos\left(\frac{2\pi}{3a}\sqrt{3}y\right) - 224$$

224

225 
$$+2V_{1,(11)}\left(\cos\left(\frac{4\pi}{3a}x-\frac{\pi}{3}\right)+2\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\right)-4V_{1,(20)}\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x+\frac{2\pi}{3}\right)+$$
  
226 
$$+4V_{1,(12)}\left(2\cos\left(\frac{2\pi}{3a}x\right)\cos\left(\frac{2\pi}{3a}\sqrt{3}y\right)-\sin\left(\frac{2\pi}{3a}x-\frac{\pi}{3}\right)\cos\left(\frac{2\pi}{3a}\sqrt{3}y\right)\right)+$$

$$227 + 2V_{1,(22)} \left( 2\cos\left(\frac{8\pi}{3a}\sqrt{3}y\right) - \cos\left(\frac{8\pi}{3a}x - \frac{2\pi}{3}\right) \right).$$
(20)

228 We need the derivatives for the forces components in dimensionless form

$$229 \qquad -\frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} + \frac{\pi}{3}\right) \cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right) \sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right) \sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right) \sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right) \sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right)\sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right)\sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right)\sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}x + \frac{\pi}{3}\right)\cos\left(\frac{4\pi}{3\tilde{a}}x + \frac{\pi}{3}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}x + \frac{\pi}{3}\right)\cos\left(\frac{4\pi}{3\tilde{a}}x + \frac{\pi}{3}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}x + \frac{\pi}{3}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{\pi}{3\tilde{a}}x + \frac{\pi}{3}\right)\cos\left(\frac{\pi}{3}x + \frac{\pi}{3}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{\pi}{3}x + \frac{\pi}{3}\right)\cos\left(\frac{\pi}{3}x + \frac{\pi}{3}\right) + \\230 \qquad -\tilde{U}_{20}' \cos\left(\frac{\pi}{3}x + \frac{\pi}{3}\right)\cos\left(\frac{\pi}{3}x + \frac{\pi}{3}\right)\cos\left(\frac{\pi}{3}x + \frac{\pi}{$$

231 
$$+\cos\left(\frac{2\pi}{3\widetilde{a}}\widetilde{x}-\frac{\pi}{6}\right)\cos\left(\frac{2\pi}{\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right)-\widetilde{U}_{22}'\sin\left(\frac{8\pi}{3\widetilde{a}}\widetilde{x}-\frac{2\pi}{3}\right),$$
 (21)

$$233 \quad -\sqrt{3}\widetilde{U}_{20}'\sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\cos\left(\frac{4\pi}{3\widetilde{a}}\widetilde{x}+\frac{2\pi}{3}\right)+\widetilde{U}_{12}'\left(2\sqrt{3}\cos\left(\frac{2\pi}{\widetilde{a}}\widetilde{x}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3}\sqrt{3}\widetilde{y}\right)-\frac{\pi}{3\widetilde{a}}\cos\left(\frac{2\pi}{3$$

234 
$$-3\sqrt{3}\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{6}\right)\sin\left(\frac{2\pi}{\tilde{a}}\sqrt{3}\tilde{y}\right) + 2\sqrt{3}\tilde{U}_{22}'\sin\left(\frac{8\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right),$$
(22)  
235 where the notations are introduced:

237 
$$\tilde{U}_{10}' = \frac{8\pi}{3\tilde{a}} \tilde{V}_{1,(10)}, \quad \tilde{U}_{11}' = \frac{8\pi}{3\tilde{a}} \tilde{V}_{1,(11)}, \quad \tilde{U}_{20}' = \frac{16\pi}{3\tilde{a}} \tilde{V}_{1,(20)}, \quad \tilde{U}_{12}' = \frac{8\pi}{3\tilde{a}} \tilde{V}_{1,(12)}, \quad \tilde{U}_{22}' = \frac{16\pi}{3\tilde{a}} \tilde{V}_{1,(22)}. \quad (23)$$

Consider as the approximation the acting forces by  $\tilde{t} = 0$ , when  $\tilde{\xi} = \tilde{x}$ . After substitution of (21) and (22) in (9), one obtains the expressions for the dimensionless forces acting on the unit of mass of particles:

$$\begin{split} \widetilde{F}_{p\xi} &= -\frac{\partial \widetilde{\varphi}}{\partial \xi} + \widetilde{U}_{10}' \sin\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{\pi}{3}\right) \cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{U}_{11}' \sin\left(\frac{4\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{\pi}{3}\right) - \\ 242 &\quad -\widetilde{U}_{20}' \cos\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) \sin\left(\frac{4\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{2\pi}{3}\right) + \widetilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\widetilde{a}}\widetilde{\xi}\right)\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right) + \\ &\quad +\cos\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{\pi}{6}\right)\cos\left(\frac{2\pi}{\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right) - \widetilde{U}_{22}' \sin\left(\frac{8\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{2\pi}{3}\right) + \widetilde{E}_{\xi}, \end{split}$$

$$\widetilde{F}_{py} &= -\frac{\partial \widetilde{\varphi}}{\partial \widetilde{y}} + \widetilde{U}_{10}' \sqrt{3}\cos\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{\pi}{3}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{U}_{11}' 2\sqrt{3}\sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) - \\ 243 &\quad -\sqrt{3}\widetilde{U}_{20}' \sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\cos\left(\frac{4\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{2\pi}{3}\right) + \widetilde{U}_{12}' \left(2\sqrt{3}\cos\left(\frac{2\pi}{\widetilde{a}}\widetilde{\xi}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) - \\ &\quad -3\sqrt{3}\sin\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{\pi}{6}\right)\sin\left(\frac{2\pi}{\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right) + 2\sqrt{3}\widetilde{U}_{22}' \sin\left(\frac{8\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{E}_{y}. \end{split}$$

244 Analogically

245

$$\widetilde{F}_{e\xi} = -\widetilde{F}_{p\xi}, \ \widetilde{F}_{ey} = -\widetilde{F}_{py}.$$
<sup>(26)</sup>

246 The forces (24)-(26) should be introduced in the system of the hydrodynamic equations (3)-(8).

Suppose that the external field intensity **E** is equal to zero. Average on  $\tilde{y}$  the obtained system of quantum hydrodynamic equations taking into account that effective hydrodynamic velocity is directed along x axis. The averaging will be realized in the limit of one hexagonal crystal cell. Carry out the integration of the left and right hand sides of the hydrodynamic equations

251 calculating the integral 
$$\frac{1}{\sqrt{3}\tilde{a}} \int_{\frac{\sqrt{3}\tilde{a}}{2}\tilde{a}}^{\frac{\sqrt{3}\tilde{a}}{2}\tilde{a}} d\tilde{y}$$
 (see Fig. 1) and taking into account that  $\frac{1}{\sqrt{3}\tilde{a}} \int_{\frac{\sqrt{3}\tilde{a}}{2}\tilde{a}}^{\frac{\sqrt{3}\tilde{a}}{2}\tilde{a}} \frac{\partial\psi}{\partial\tilde{y}} d\tilde{y} = 0$ 

252 because of system symmetry for arbitrary function  $\Psi$ , characterizing the state of the physical

- 253 system. We suppose therefore that by averaging all physical values, characterizing the state of the
- 254 physical system do not depend on  $\tilde{y}$ .
- As result we have the following system of equations:
- 256 Dimensionless Poisson equation for the self-consistent potential  $\tilde{\varphi}$  of the electric field:

$$257 \qquad \frac{\partial^2 \widetilde{\varphi}}{\partial \widetilde{\xi}^2} = -4\pi R \left\{ \frac{m_e}{m_p} \left[ \widetilde{\rho}_p - \frac{m_e H}{m_p \widetilde{u}^2} \frac{\partial}{\partial \widetilde{\xi}} \left( \widetilde{\rho}_p \left( \widetilde{u} - 1 \right) \right) \right] - \left[ \widetilde{\rho}_e - \frac{H}{\widetilde{u}^2} \frac{\partial}{\partial \widetilde{\xi}} \left( \widetilde{\rho}_e \left( \widetilde{u} - 1 \right) \right) \right] \right\}.$$

$$(27)$$

- 258
- 259 Continuity equation for the positive particles:

$$\frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{p} (1 - \tilde{u}) \right] + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{p} (\tilde{u} - 1)^{2} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \left( -\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) \right] \right\} = 0$$

$$(28)$$

262 Continuity equation for electrons:

263

$$\frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{e} (1 - \tilde{u}) \right] + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{e} (\tilde{u} - 1)^{2} \right] \right\} + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{e} - \tilde{\rho}_{e} E \left( \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right] \right\} = 0$$

$$(29)$$

265 Momentum equation for the movement along the *x* direction:266

$$\frac{\partial}{\partial \tilde{\xi}} \left\{ \left( \tilde{\rho}_{p} + \tilde{\rho}_{e} \right) \tilde{u} \left( \tilde{u} - 1 \right) + \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} + \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \right\} - \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \left( -\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) - \tilde{\rho}_{e} E \left( \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) + \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right\} + \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right\} + \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right\} + \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right\} + \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) \right\} + \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \frac{1}{2} \left\{ \frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left( \frac{\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left( \frac{\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) \right\} \right\}$$

$$+\frac{m_{e}}{m_{p}}\frac{\partial}{\partial\xi}\left\{\frac{H}{\tilde{\mu}^{2}}\left[\frac{\partial}{\partial\xi}\left[2\frac{V_{a_{0}}^{2}}{u_{0}^{2}}\tilde{p}_{p}\left(1-\tilde{u}\right)-\tilde{p}_{p}\tilde{u}\left(1-\tilde{u}\right)^{2}\right)-\frac{m_{e}}{m_{p}}\tilde{\rho}_{p}\left(1-\tilde{u}\right)E\left(-\frac{\partial\tilde{\varphi}}{\partial\xi}+\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right)\right]\right\}+$$

$$+\frac{\partial}{\partial\xi}\left[\frac{H}{\tilde{\mu}^{2}}\left[\frac{\partial}{\partial\xi}\left[2\frac{V_{o_{e}}^{2}}{u_{0}^{2}}\tilde{p}_{e}\left(1-\tilde{u}\right)-\tilde{\rho}_{e}\tilde{u}\left(1-\tilde{u}\right)^{2}\right)-\frac{\tilde{\rho}_{e}\left(1-\tilde{u}\right)E\left(-\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)+\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right)\right]\right\}+$$

$$+\frac{H}{\tilde{u}^{2}}E\left(\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right)\left(\frac{\partial}{\partial\tilde{\xi}}\left(\tilde{\rho}_{p}\left(\tilde{u}-1\right)\right)\right)+$$

$$+\frac{H}{\tilde{u}^{2}}E\left(\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)+\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right)\left(\frac{\partial}{\partial\tilde{\xi}}\left(\tilde{\rho}_{p}\left(\tilde{u}-1\right)\right)\right)-$$

$$270 -\frac{m_{e}}{m_{p}}\frac{\partial}{\partial\tilde{\xi}}\left\{\frac{H}{\tilde{u}^{2}}\frac{V_{o_{e}}^{2}}{u_{0}^{2}}\frac{\partial}{\partial\tilde{\xi}}\left(\tilde{\rho}_{p}\tilde{u}\right)\right\}-\frac{\partial}{\partial\tilde{\xi}}\left\{\frac{H}{\tilde{u}^{2}}\frac{V_{o_{e}}^{2}}{u_{0}^{2}}\frac{\partial}{\partial\tilde{\xi}}\left(\tilde{\rho}_{p}\tilde{u}\right)\right\}-\frac{\partial}{\partial\tilde{\xi}}\left\{\frac{H}{\tilde{u}^{2}}\frac{V_{o_{e}}^{2}}{u_{0}^{2}}\frac{\partial}{\partial\tilde{\xi}}\left(\tilde{\rho}_{e}\tilde{u}\right)\right\}+$$

$$\left\{\frac{H}{\tilde{u}^{2}}\left[\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right]\tilde{\rho}_{p}\tilde{u}\right]\right\}+$$

$$\left\{\frac{H}{\tilde{u}^{2}}\left[\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right]\tilde{\rho}_{p}\tilde{u}\right]\right\}+$$

$$\left\{\frac{H}{\tilde{u}^{2}}\left[\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right]\tilde{\rho}_{p}\tilde{u}\right]\right\}+$$

$$\left\{\frac{H}{\tilde{u}^{2}}\left[\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}-\tilde{U}_{11}^{\prime}\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)+\tilde{U}_{22}^{\prime}\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right]\tilde{\rho}_{p}\tilde{u}\right]\right\}=0$$

$$\frac{272}{273}$$
Energy equation for the positive particles:
$$\left\{\frac{1}{\tilde{u}^{2}}\left[\frac{1}{\tilde{u}^{2}}\left[\frac{2}{\tilde{u}^{2}}\tilde{u}\right]^{\prime}$$

$$\frac{\partial}{\partial \tilde{\xi}} \left[ \tilde{\rho}_{p} \tilde{u}^{2} (\tilde{u}-1) + 5 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u} - 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \right] - \frac{2m_{e}}{m_{p}} \tilde{\rho}_{p} E \left( -\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3}\right) \right) \tilde{u} + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{m_{e}}{m_{p}} \left[ \frac{\partial}{\partial \tilde{\xi}} \left( -\tilde{\rho}_{p} \tilde{u}^{2} (1-\tilde{u})^{2} + 7 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u} (1-\tilde{u}) + 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} (\tilde{u}-1) - \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u}^{2} - 5 \frac{V_{0p}^{4}}{u_{0}^{4}} \frac{\tilde{p}_{p}^{2}}{\tilde{\rho}_{p}} \right) + E \left( -2 \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} \tilde{u} (1-\tilde{u}) + \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} \tilde{u}^{2} + 5 \frac{m_{e}}{m_{p}} \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} \right) \left( -\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \frac{\tilde{u}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3}\right)}{\tilde{u}_{0}^{2}} \right) \right) \right\} + 2 \frac{H}{\tilde{u}^{2}} E \left( \frac{m_{e}}{m_{p}} \right)^{2} \left[ -\frac{\partial}{\partial \tilde{\xi}} (\tilde{\rho}_{p} \tilde{u} (1-\tilde{u})) + \frac{V_{0p}^{2}}{\tilde{\rho}_{p}} \tilde{\ell}_{11} \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3}\right) \right) \right] \right\} - 2 \frac{H}{\tilde{u}^{2}} E \left( \frac{m_{e}}{m_{p}} \right)^{2} \left[ -\frac{\partial}{\partial \tilde{\xi}} (\tilde{\rho}_{p} \tilde{u} (1-\tilde{u})) + \frac{V_{0p}^{2}}{\tilde{\rho}_{p}} \tilde{\rho}_{p} \right] \left( -\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3}\right) \right) - 278$$

$$-2\frac{H}{\tilde{u}^{2}}E^{2}\left(\frac{m_{e}}{m_{p}}\right)^{3}\tilde{\rho}_{p}\left[\left(-\frac{\partial\tilde{\varphi}}{\partial\xi}+\tilde{U}_{11}'\sin\left(\frac{4\pi}{3\tilde{a}}\xi-\frac{\pi}{3}\right)-\tilde{U}_{22}'\sin\left(\frac{8\pi}{3\tilde{a}}\xi-\frac{2\pi}{3}\right)\right)^{2}+\right.\\\left.+\frac{1}{2}\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\xi+\frac{\pi}{3}\right)+6\tilde{U}_{12}'\sin\left(\frac{2\pi}{\tilde{a}}\xi\right)\right)^{2}+\frac{1}{2}\left(\tilde{U}_{12}'\right)^{2}\cos^{2}\left(\frac{2\pi}{3\tilde{a}}\xi-\frac{\pi}{6}\right)+\right.\\\left.+\frac{1}{2}\left(\tilde{U}_{02}'\right)^{2}\sin^{2}\left(\frac{4\pi}{3\tilde{a}}\xi+\frac{2\pi}{3}\right)-\frac{4}{3\pi}\tilde{U}_{02}'\sin\left(\frac{4\pi}{3\tilde{a}}\xi+\frac{2\pi}{3}\right)\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\xi+\frac{\pi}{3}\right)+6\tilde{U}_{12}'\sin\left(\frac{2\pi}{\tilde{a}}\xi\right)\right)-\right.\\\left.-\frac{12}{5\pi}\tilde{U}_{02}'\tilde{U}_{12}'\sin\left(\frac{4\pi}{3\tilde{a}}\xi+\frac{2\pi}{3}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\xi-\frac{\pi}{6}\right)+\frac{3}{2}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\xi+\frac{\pi}{3}\right)+2\tilde{U}_{12}'\cos\left(\frac{2\pi}{\tilde{a}}\xi\right)\right)^{2}+\right.\\\left.+\frac{3}{2}\left(2\tilde{U}_{11}'-\tilde{U}_{02}'\cos\left(\frac{4\pi}{3\tilde{a}}\xi+\frac{2\pi}{3}\right)\right)^{2}+\frac{27}{2}\left(\tilde{U}_{12}'\right)^{2}\sin^{2}\left(\frac{2\pi}{3\tilde{a}}\xi-\frac{\pi}{6}\right)+6\tilde{U}_{22}'\right)^{2}+\right.\\\left.+\frac{8}{\pi}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\xi+\frac{\pi}{3}\right)+2\tilde{U}_{12}'\cos\left(\frac{2\pi}{\tilde{a}}\xi\right)\right)\left(2\tilde{U}_{11}'-\tilde{U}_{02}'\cos\left(\frac{4\pi}{3\tilde{a}}\xi+\frac{2\pi}{3}\right)\right)-\right.\\\left.-\frac{96}{15\pi}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\xi+\frac{\pi}{3}\right)+2\tilde{U}_{12}'\cos\left(\frac{2\pi}{\tilde{a}}\xi\right)\right)\tilde{U}_{22}'-\right.\\\left.279$$

$$\left.-\frac{72}{5\pi}\tilde{U}_{12}'\left(2\tilde{U}_{11}'-\tilde{U}_{02}'\cos\left(\frac{4\pi}{3\tilde{a}}\xi+\frac{2\pi}{3}\right)\right)\sin\left(\frac{2\pi}{3\tilde{a}}\xi-\frac{\pi}{6}\right)-\frac{288}{7\pi}\tilde{U}_{12}'\tilde{U}_{22}'\sin\left(\frac{2\pi}{3\tilde{a}}\xi-\frac{\pi}{6}\right)\right]=\right.$$

$$\left.280$$

$$\left.-\frac{\tilde{u}^{2}}{Hu_{0}^{2}}\left(V_{0p}^{2}\tilde{p}_{p}-\tilde{p}_{e}V_{0e}^{2}\left(1+\frac{m_{p}}{m_{e}}\right)\right)\right.$$
(31)

282 Energy equation for electrons:283

$$\frac{\partial}{\partial \xi} \left[ \tilde{\rho}_{e} \tilde{u}^{2} (\tilde{u} - 1) + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \tilde{u} - 3 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \right] - 2\tilde{\rho}_{e} \tilde{u} E \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi} - \frac{2\pi}{3}\right) \right) + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{\partial}{\partial \xi} \left( - \tilde{\rho}_{e} \tilde{u}^{2} (1 - \tilde{u})^{2} + 7 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \tilde{u} (1 - \tilde{u}) + 3 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} (\tilde{u} - 1) - \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \tilde{u}^{2} - 5 \frac{V_{0e}^{4}}{u_{0}^{4}} \frac{\tilde{p}_{e}^{2}}{\tilde{\rho}_{e}} \right) + E \left( -2\tilde{\rho}_{e} \tilde{u} (1 - \tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi} - \frac{2\pi}{3}\right) \right) \right] \right\} + 286 + E \left( -2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1 - \tilde{u})) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi} - \frac{2\pi}{3}\right) \right) \right] \right] + 286 + E \left( -2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1 - \tilde{u})) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi} - \frac{2\pi}{3}\right) \right) \right] - 286 + E \left( -2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1 - \tilde{u})) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi} - \frac{2\pi}{3}\right) \right) \right] - 286 + E \left( -2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1 - \tilde{u})) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi} - \frac{2\pi}{3}\right) \right) \right) - 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} } \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{U}_{22}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) \right) \right) \right)$$

$$-2E^{2}\frac{H}{\tilde{u}^{2}}\tilde{\rho}_{\epsilon}\left[\left(-\frac{\partial\tilde{\varphi}}{\partial\xi}+\tilde{U}_{11}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}'\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right)^{2}+\right.\\ +\frac{1}{2}\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)+6\tilde{U}_{12}'\sin\left(\frac{2\pi}{\tilde{a}}\tilde{\xi}\right)\right)^{2}+\frac{1}{2}\left(\tilde{U}_{12}'\right)^{2}\cos^{2}\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{6}\right)+\\ +\frac{1}{2}\left(\tilde{U}_{02}'\right)^{2}\sin^{2}\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}+\frac{2\pi}{3}\right)-\frac{4}{3\pi}\tilde{U}_{02}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}+\frac{2\pi}{3}\right)\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)+6\tilde{U}_{12}'\sin\left(\frac{2\pi}{\tilde{a}}\tilde{\xi}\right)\right)-\\ -\frac{12}{5\pi}\tilde{U}_{02}'\tilde{U}_{12}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}+\frac{2\pi}{3}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{6}\right)+\frac{3}{2}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)+2\tilde{U}_{12}'\cos\left(\frac{2\pi}{\tilde{a}}\tilde{\xi}\right)\right)^{2}+\\ +\frac{3}{2}\left(2\tilde{U}_{11}'-\tilde{U}_{02}'\cos\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}+\frac{2\pi}{3}\right)\right)^{2}+\frac{27}{2}\left(\tilde{U}_{12}'\right)^{2}\sin^{2}\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{6}\right)+6\tilde{U}_{22}'^{2}+\\ +\frac{8}{\pi}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)+2\tilde{U}_{12}'\cos\left(\frac{2\pi}{\tilde{a}}\tilde{\xi}\right)\right)\left(2\tilde{U}_{11}'-\tilde{U}_{02}'\cos\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}+\frac{2\pi}{3}\right)\right)-\\ -\frac{96}{15\pi}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)+2\tilde{U}_{12}'\cos\left(\frac{2\pi}{\tilde{a}}\tilde{\xi}\right)\right)\tilde{U}_{22}'-\\ -\frac{72}{5\pi}\tilde{U}_{12}'\left(2\tilde{U}_{11}'-\tilde{U}_{02}'\cos\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}+\frac{2\pi}{3}\right)\right)\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{6}\right)-\frac{288}{7\pi}\tilde{U}_{12}'\tilde{U}_{22}'\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{6}\right)\right]=\\ =-\frac{\tilde{u}^{2}}{Hu_{0}^{2}}\left(V_{0e}^{2}\tilde{\rho}_{e}-V_{0p}^{2}\tilde{\rho}_{p}\left(1+\frac{m_{p}}{m_{e}}\right)\right)$$
(32)

288

287

## **3. Estimations of the numerical parameters.**

We need estimations for the numerical values of dimensionless parameters for solutions of the hydrodynamic equations (27) - (32). In its turn these parameters depend on choosing of the independent scales physical values. Analyze the independent scales for the physical problem under consideration.

The surface electron density in graphene is about  $\tilde{n}_e \approx 10^{10} cm^{-2}$ , the thickness of the graphene layer is equal to ~ 1 nm. Then the electron concentration consists  $n_e \approx 10^{17} cm^{-3}$ , and the density for the electron species  $\rho_e = m_e n_e \approx 10^{-10} g/cm^3$  which leads to the scale  $\rho_0 = 10^{-10} g/cm^3$ . For numerical solutions of the hydrodynamic equations (27)-(32) we need Cauchy conditions, obviously in the typical for grapheme conditions the estimation  $\tilde{\rho}_e \sim 1$  is valid which can be used as the condition by  $\tilde{\xi} = 0$ .

The process of the carbon atoms polarization leads to displacement of the atoms from the regular chain and to the creation of the "effective" positive particles which concentration  $n_p \approx n_e$ . Masses of these particles is about the mass of the carbon atom  $m_p \approx 2 \cdot 10^{-23} e$ . Then,  $\frac{L}{T} = \frac{m_e}{m_p} \approx 5 \cdot 10^{-5}$ ;  $\rho_p = m_p n_p \approx 2 \cdot 10^{-6} g/cm^3$  and by the choosed scale for the density  $\rho_0$  we

305 have 
$$\tilde{\rho}_p \sim 2 \cdot 10^4$$
.

306 Going to the scales for thermal velocities for electrons and the positive particles we have 307 by $T=300^{\circ}$ K:

308 
$$V_{0e} \sim \sqrt{\frac{k_B T}{m_e}} \approx 6.4 \cdot 10^6 \, cm/c$$
, take the scale  $V_{0e} = 5 \cdot 10^6 \, cm/s$ ;

309 
$$V_{0p} \sim \sqrt{\frac{k_B T}{m_p}} \approx 4.5 \cdot 10^4 \, c_M/c$$
, take the scale  $V_{0p} = 5 \cdot 10^4 \, c_M/s$ 

310 The theoretical mobility in graphene reaches up to  $10^6 cm^2/V \cdot s$ . Let us use the scale

311 
$$u_0 = 5 \cdot 10^6 \, cm/s$$
. Then  $N = \frac{V_{0e}^2}{u_0^2} = 1$ ,  $P = \frac{V_{0p}^2}{u_0^2} = 10^{-4}$ 

Let us estimate the parameters E and R. For this estimation we need the scale  $\varphi_0$ . Admit 312  $\varphi_0 \approx \delta \frac{e}{a}$ , where  $\delta$  is a "shielding coefficient". Naturally to take  $x_0 = a = 0.142$  nm (see Fig. 1)- as 313 314 the length scale, then  $\tilde{a} = 1$ . In the situation of a uncertainty in  $\varphi_0$  choosing let us consider two 315 limit cases: 316 317 δ~1. Then  $E = \frac{e\varphi_0}{m u_0^2} \sim 1000$ ,  $R = \frac{e\rho_0 x_0^2}{m_s \varphi_0} \sim 3 \cdot 10^{-7}$ . 318 319 2) δ=0.0001. Then  $E = \frac{e\varphi_0}{m_e u_0^2} \sim 0.1$ ,  $R = \frac{e\rho_0 x_0^2}{m_e \varphi_0} \sim 3.10^{-3}$ . 320 321 Consider the terms describing the lattice influence. We should estimate the coefficients (23) using  $\varphi_0$  as the scale for the potential  $V, V = \varphi_0 \tilde{V}$ . Three possible cases under consideration: 322 1)  $V \sim \varphi_0$ 323 We choose  $U = \tilde{U}'_{10} \sim 10$ ,  $F = \tilde{U}'_{11} \sim 10$ ,  $J = \tilde{U}'_{20} \sim \pm 5$ ,  $B = \tilde{U}'_{12} \sim \pm 2,5$ ,  $G = \tilde{U}'_{22} \sim \pm 5$ . 324 325 In this case the coefficients of "the second order" are less than the coefficients of "the first order." 2)  $V \prec \varphi_0$  (The small influence of the lattice), 326 We choose  $U = \tilde{U}'_{10} \sim 0.1$ ,  $F = \tilde{U}'_{11} \sim 0.1$ ,  $J = \tilde{U}'_{20} \sim 0.05$ ,  $B = \tilde{U}'_{12} \sim 0.025$ ,  $G = \tilde{U}'_{22} \sim 0.05$ . 327 3)  $V \succ \varphi_0$  (The great influence of the lattice), 328 We choose  $U = \tilde{U}'_{10} \sim 1000$ ,  $F = \tilde{U}'_{11} \sim 1000$ ,  $J = \tilde{U}'_{20} \sim 500$ ,  $B = \tilde{U}'_{12} \sim 250$ ,  $G = \tilde{U}'_{22} \sim 500$ . 329 Estimate parameter  $H = \frac{N_R \hbar}{m_x x_0 u_0}$  for two limit cases: 330 1)  $N_R = 1$ , then  $H \sim 15$ . 331 2)  $N_R = 100$ , then  $H \sim 1500$ . 332

333	Initial conditions demand also the estimations for the quantum electron pressure and the											
334	pressure for the positive species. For the electron pressure we have $p_e = \rho_0 V_{0e}^2 \tilde{p}_e$ and using for the											
335	scale estimation $p_e = n_e k_B T \sim n_e m_e V_{oe}^2 = \rho_e V_{oe}^2 \sim \rho_0 V_{oe}^2$ , one obtains $\tilde{p}_e \sim 1$ . Analogically for the										gically for the	
336	positive particles $p_p = \rho_0 V_{0p}^2 \tilde{p}_p$ , and using $p_p = n_p k_B T \sim n_p m_p V_{op}^2 = \rho_p V_{0p}^2$ , we have											
337	$p_{p} \sim 2 \cdot 10^{4} \rho_{0} V_{0p}^{2}, \ \tilde{p}_{p} \sim 2 \cdot 10^{4}.$											
338	Tables 1, 2 contain the initial conditions and parameters which were not varied by the											
339	numerical modeling.											
340												
341	Table 1. Initial conditions.											
	$\widetilde{ ho}_{_{e}}(0)$	${\widetilde  ho}_{_p}(0)$	$\widetilde{\varphi}(0)$	${\widetilde p}_{e}(0)$	$\widetilde{p}_{p}(0)$	$rac{\partial \widetilde{ ho}_{_{e}}}{\partial \widetilde{\xi}}(0)$	$rac{\partial {\widetilde  ho}_{_p}}{\partial {\widetilde \xi}}($	(0) $\left  \frac{\partial \theta}{\partial \theta} \right $	$\frac{\widetilde{p}}{\widetilde{\xi}}(0)$	$\frac{\partial \widetilde{p}_{e}}{\partial \widetilde{\xi}}(0)$	$\frac{\partial \widetilde{p}_{p}}{\partial \widetilde{\xi}}$	- (0)
	1	$2 \cdot 10^4$	1	1	$2 \cdot 10^4$	0	0	0	Ĝ	0	0	
342												
343	Table 2. Constant parameters .											
	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$											
344												
345	Table 3 contains parameters (for the six different cases) which were varied by the numerical											
346	modeling.											
347	Table 3. Varied parameters.											
348												
		N N	Variant.	N <u>∘</u> E	R	Н	U	F	J	В	G	
		1		0.1	0.003	15	10	10	5	2.5	5	
			2	0.1	0.003	15	0.1	0.1	0.05	0.025	0.05	
			3	0.1	0.003	15	10	10	-5	-2.5	-5	
			1	1000	3.10	7 15	10	10	5	2.5	5	

In the present time there no the foolproof methods of the calculations of the potential lattice forces in graphene. In the following mathematical modeling the strategy is taken consisting in the vast variation of the parameters defining the evolution of the physical system.

2.5

0.003

0.003

0.1

0.1

- **4. Results of the mathematical modeling without the external electric field.**
- The calculations are realized on the basement of equations (27)-(32) by the initial conditions and parameters containing in the Tables 1 – 3. Now we are ready to display the results of the mathematical modeling realized with the help of Maple (the versions Maple 9 or more can be used). The system of generalized hydrodynamic equations (27) - (32) have the great possibilities of mathematical modeling as result of changing of Cauchy conditions and parameters describing the character features of initial perturbations which lead to the soliton formation.
- The following Maple notations on figures are used: r- density  $\tilde{\rho}_p$ , s density  $\tilde{\rho}_e$ , u- velocity  $\tilde{u}$  (solid black line), p - pressure  $\tilde{p}_p$  (black dashed line), q - pressure  $\tilde{p}_e$  and v - self consistent potential  $\tilde{\varphi}$ . Explanations placed under all following figures, Maple program contains Maple's notations - for example, the expression D(u)(0) = 0 means in the usual notations  $\frac{\partial \tilde{u}}{\partial \xi}(0) = 0$ ,
- 365 independent variable t responds to  $\tilde{\xi}$ .

Important to underline that no special boundary conditions were used for all following cases. The aim of the numerical investigation consists in the discovery of the soliton waves as a product of the self-organization of matter in graphene. It means that the solution should exist only in the restricted domain of the 1D space and the obtained object in the moving coordinate system  $(\tilde{\xi} = \tilde{x} - \tilde{t})$  has the constant velocity  $\tilde{u} = 1$  for all parts of the object. In this case the domain of the solution existence defines the character soliton size. The following numerical results demonstrate the realization of mentioned principles.

Figures 2 - 9 reflect the result of calculations for Variant 1 (Table 3) in the first and the second approximations. In the first approximation the terms of series (18) with  $|g_1| \le 1$ ,  $|g_2| \le 1$ (then coefficients *U* and *F*) were taken into account. The second approximation contains all terms of the series (18) with  $|g_1| \le 2$ ,  $|g_2| \le 2$  (then coefficients *U*, *F*, *J*, *B* and *G*).





400 the negative charge distributes over the entire soliton domain (Figs. 2, 6), but the negative charge

401 density increases to the edges of the soliton. Therefore the soliton structure reminds the 1D atom402 with the positive nuclei and the negative shell.

403 The self-consistent potential  $\tilde{\varphi}$  is practically constant in the soliton boundaries, (Figs. 4, 8). 404 The small grows of the positive particles pressure exists in the *x* direction. This effect can be 405 connected with the hydrodynamic movement along *x* and "the reconstruction" of the polarized 406 particles in the soliton front.

407 Comparing the figures 2 - 5 and 6 - 9 we conclude that the calculation results in the first 408 and the second approximation do not vary significantly. Seemingly significant difference of figures 409 2 and 6 on the edges of the domain has not the physical sense because corresponds to the regions 410 where  $u \neq const$ . Then the restriction of two successive approximations is justified. Along with it 411 the question about the convergence of the series lives open because the first and the second 412 approximations include only the restricted quantity of terms of the infinite series with the 413 coefficients known with the small accuracy.

Figures 10 - 15 show the results of calculations responding to Variant 3 (Table 3). In the first approximation Variant 3 is identical to Variant 1 (coefficients J = B = G = 0) and only the results of the second approximation are delivered. These calculations are more complicated in the numerical realization and all curves are imaged separately, (Figures 10 – 15).





433 of soliton is observed because by  $\tilde{\xi} \prec 0$  the velocity  $\tilde{u}$  is not constant. Then this kind of potential 434 for lattice is not favorable for creation of the super-conducting structures.

435 Variant 2 (Table 3) correspond to diminishing of the lattice potential in 100 times by the 436 same practically self-consistent potential, (see figures 16 - 23).





460 the self-consistent potential plays the basic role in the soliton formation.

461 Let us analyze now the influence of H - parameter, practically the influence of the non-462 locality parameter. Figures 24 - 31 (Variant 5) correspond to increasing of the parameter H in 100 463 times in comparison with Variant 1.





488 figures 6 and 28) in the second approximation leads to conclusion that the region (where the 489 velocity  $\tilde{u}$  is constant) has practically the same size.

Consider now the calculations responding to Variant 4 (Table 3). Increasing in  $10^4$  times of 490 491 the scale  $\varphi_0$  denotes increasing the self consistent potential and the lattice potential introduced in 492 the process of the mathematical modeling. This case leads to the drastic diminishing of the soliton 493 size. Figures 32 - 35 demonstrate that in the calculations of the first approximation the soliton size is  $\sim 10^{-4} a = 1.42 \cdot 10^{-12} cm$  and exceeds the nuclei size only in several times. The positive kernel of 494 the soliton decreasing in the less degree and occupies now the half of the soliton size. It is no 495 496 surprise because the low boundary of this kernel size is the character size of the nuclei. Application 497 of the second approximation for the lattice potential function in the mathematical modeling leads to 498 the significant soliton deformation but the same soliton size (see figures 36-39).







521 deformation in the second approximation (see figures 45 – 48). Figure 41 demonstrate the 522 extremely high accuracy of the soliton stability, the velocity fluctuation inside the soliton is only 523  $\sim 10^{-16} \tilde{u}$ .



527





- 545 (the second approximation, Variant 6).
- 546

# 547 **5.** Results of the mathematical modeling with the external electric field.

Let us consider now the results of the mathematical modeling with taking into account the intensity of the external electric field which does not depend on y. In this case the solution of the hydrodynamic system (3) – (8) should be found. After averaging and in the moving coordinate system it leads to the following equations written in the first approximation (compare with the system (27) – (32)):

$$\begin{aligned} \frac{\partial^{2} \tilde{\varphi}}{\partial \xi^{2}} &= -4\pi R \bigg\{ \frac{m_{r}}{m_{p}} \bigg[ \tilde{\rho}_{p} - \frac{m_{r}H}{m_{p}} \frac{\partial}{\partial \xi} \overline{\xi} \left( \tilde{\rho}_{p} \left( \tilde{u} - 1 \right) \right) \bigg] - \bigg[ \tilde{\rho}_{r} - \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} \overline{\xi} \left( \tilde{\rho}_{r} \left( \tilde{u} - 1 \right) \right) \bigg] \bigg\}. \end{aligned}$$
(33)  

$$\begin{aligned} \frac{\partial}{\partial \xi} \bigg[ \tilde{\rho}_{r} \left( 1 - \tilde{u} \right) \bigg] + \frac{m_{r}}{m_{p}} \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} \bigg[ \tilde{\rho}_{p} \left( \tilde{u} - 1 \right)^{2} \bigg] \bigg\} + \frac{m_{r}}{m_{p}} \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{u_{o}^{2}} \overline{\rho}_{p} - \bigg( \frac{\partial}{\tilde{u}^{2}} - \frac{\partial}{\tilde{u}^{2}} \overline{\rho}_{p} \left( \tilde{u} - 1 \right)^{2} \bigg] \bigg\} + \frac{m_{r}}{m_{p}} \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{u_{o}^{2}} \overline{\rho}_{p}^{2} \tilde{\rho}_{p} - \bigg( \frac{\partial}{\tilde{u}^{2}} - \frac{\partial}{\tilde{u}^{2}} \overline{\xi} + \tilde{U}_{11}^{\prime} \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{E}_{0} \bigg) \bigg] \bigg\} = 0 \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial \xi} \bigg[ \tilde{\rho}_{r} \left( 1 - \tilde{u} \right) \bigg] + \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} \bigg[ \tilde{\rho}_{r} \left( \tilde{u} - 1 \right)^{2} \bigg] \bigg\} + \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \bigg[ \frac{V_{0}}{u_{o}} \frac{\partial}{\partial \xi} \tilde{\rho}_{p} - \bigg( \frac{\partial}{\tilde{u}^{2}} - \frac{\partial}{\tilde{u}^{2}} \overline{\rho}_{p} \right) \bigg\} \\ - \tilde{\rho}_{r} E \bigg\{ \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}^{\prime} \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{E}_{0} \bigg] \bigg] \bigg\} = 0 \end{aligned}$$

$$\begin{aligned} \text{Momentum equation for the x direction:} \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial \xi} \bigg\{ \bigg( \tilde{\rho}_{r} + \tilde{\rho}_{r} \bigg) \tilde{u} \left( \tilde{u} - 1 \bigg) + \frac{V_{0}^{2}}{u_{o}^{2}} \tilde{\rho}_{r} - \frac{\tilde{E}_{0}}{\tilde{u}_{o}^{2}} \right) \bigg\} \\ - \tilde{\rho}_{r} E \bigg\{ \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}^{\prime} \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{E}_{0} \bigg\} \bigg\} = 0 \end{aligned}$$

$$\begin{aligned} \text{Momentum equation for the x direction:} \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial \xi} \bigg\{ \bigg( \tilde{\rho}_{r} + \tilde{\rho}_{r} \bigg) \tilde{u} \left( \tilde{u} - 1 \bigg) + \frac{V_{0}^{2}}{u_{o}^{2}} \tilde{\rho}_{r} - \frac{\pi}{3} \bigg\} + \tilde{E}_{0} \bigg\} - \\ - \tilde{\rho}_{r} E \bigg\{ \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}^{\prime} \sin \left( \frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \bigg\} - \tilde{E}_{0} \bigg\} + \\ + \frac{m_{r}}}{m_{r}} \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \bigg\{ \frac{\partial}{\partial \xi} \bigg\{ 2 \frac{V_{0}^{2}}{u_{o}^{2}}} \tilde{\rho}_{r} \left( 1 - \tilde{u} \bigg) - \tilde{\rho}_{r} \left( 1 - \tilde{u} \bigg) - \tilde{\rho}_{r} \left( 1 - \tilde{u} \bigg) \bigg\} \bigg\} + \\ + \frac{\partial}{\partial \xi} \bigg\{ \bigg\{ \frac{H}{\tilde{u}^{2}} \bigg\{ \frac{\partial}{\partial \xi} \bigg\{ 2 \frac{V_{0}^{2}}}{u_{o}^{2}}} \tilde{\rho}_{r} \left( 1 - \tilde{u} \bigg) - \tilde{\rho}_{r} \left( 1 - \tilde{u} \bigg) - \tilde{\rho}_{r} \left( 1 - \tilde{u} \bigg) \bigg\} \bigg\} \bigg\} \bigg\} \bigg\} \bigg\} \bigg\} + \\ \\ + \frac{\partial}{\partial \xi} \bigg\{ \frac{H}{\tilde{u}^{2}} \bigg\{ \frac{\partial}{\partial \xi} \bigg\{ 2 \frac{V_{0}^{2}}}{u_$$

Dimensionless Poisson equation for the self-consistent electric field:

$$52^{-1} = \frac{m_{e}}{m_{p}} \frac{\partial}{\partial\xi} \left\{ \frac{H}{\tilde{u}^{2}} \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial\xi} (\tilde{p}_{p}\tilde{u}) \right\} - \frac{\partial}{\partial\xi} \left\{ \frac{H}{\tilde{u}^{2}} \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial\xi} (\tilde{p}_{e}\tilde{u}) \right\} + \\ + \left(\frac{m_{e}}{m_{p}}\right)^{2} E \frac{\partial}{\partial\xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \left( -\frac{\partial\tilde{\varphi}}{\partial\xi} + \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{E}_{0} \right) \tilde{\rho}_{p}\tilde{u} \right] \right\} + \\ + E \frac{\partial}{\partial\xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \left( \frac{\partial\tilde{\varphi}}{\partial\xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) - \tilde{E}_{0} \right) \tilde{\rho}_{e}\tilde{u} \right] \right\} = 0$$

$$570 \qquad \text{Energy equation for the positive particles:}$$

$$571 \qquad \frac{\partial}{\partial\xi} \left[ \tilde{\rho}_{p}\tilde{u}^{2}(\tilde{u}-1) + 5 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p}\tilde{u} - 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p} \right] - 2 \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \left( -\frac{\partial\tilde{\varphi}}{\partial\xi} + \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3}\right) + \tilde{E}_{0} \right) \tilde{u} + \\ + \frac{\partial}{\partial\xi} \left\{ \frac{H}{\tilde{u}^{2}} \frac{m_{e}}{m_{p}} \left[ \frac{\partial}{\partial\xi} \left( -\tilde{\rho}_{p}\tilde{u}^{2}(1-\tilde{u})^{2} + 7 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p}\tilde{u}^{2}(1-\tilde{u}) + 3 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p}(\tilde{u}-1) - \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p}\tilde{u}^{2} - 5 \frac{V_{0p}^{4}}{u_{0}^{4}} \frac{\tilde{\rho}_{p}^{2}}{\tilde{\rho}_{p}} \right) + \\ 573 \qquad + E \left( -2 \frac{m_{e}}{m_{p}} \tilde{\rho}_{p}\tilde{u}^{2}(1-\tilde{u}) + \frac{m_{e}}{m_{p}} \tilde{\rho}_{p}\tilde{u}^{2} + 5 \frac{m_{e}}{m_{p}} \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p} \right) \left( -\frac{\partial\tilde{\varphi}}{\partial\xi} + \frac{\tilde{\omega}}{U}_{11} \sin\left( \frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3} \right) + \tilde{E}_{0} \right) \right] \right\} + 2 \frac{H}{\tilde{u}^{2}} E \left( \frac{m_{e}}{m_{p}} \right)^{2} \left[ -\frac{\partial}{\partial\xi} (\tilde{\rho}_{p}\tilde{u}(1-\tilde{u})) + \frac{V_{0p}^{2}}{\partial\xi} \tilde{\rho}_{p} \right) \left( -\frac{\partial\tilde{\varphi}}{\partial\xi} + \tilde{U}_{11}' \sin\left( \frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3} \right) + \tilde{E}_{0} \right) - \\ 574 \qquad + \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial\xi} \tilde{\rho}_{p} \tilde{\rho}_{p} \right] \left( -\frac{\partial\tilde{\varphi}}{\partial\xi} + \tilde{U}_{11}' \sin\left( \frac{4\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{3} \right) + \tilde{E}_{0} \right) - \\ 575 \qquad$$

 $-2\frac{H}{\tilde{u}^{2}}E^{2}\left(\frac{m_{e}}{m_{p}}\right)^{3}\tilde{\rho}_{p}\left[\left(-\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}+\tilde{U}_{11}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)+\tilde{E}_{0}\right)^{2}+\frac{1}{2}\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right)^{2}+\frac{3}{2}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right)^{2}+6\left(\tilde{U}_{11}'\right)^{2}+\frac{16}{\pi}\left(\tilde{U}_{10}'\tilde{U}_{11}'\right)\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right]= 577 = -\frac{\tilde{u}^{2}}{Hu_{0}^{2}}\left(V_{0p}^{2}\tilde{p}_{p}-\tilde{p}_{e}V_{0e}^{2}\left(1+\frac{m_{p}}{m_{e}}\right)\right)$ (37)

Energy equation for electrons:

$$581 \qquad \frac{\partial}{\partial \xi} \left[ \tilde{\rho}_{e} \tilde{u}^{2} (\tilde{u}-1) + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \tilde{u} - 3 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \right] - 2 \tilde{\rho}_{e} \tilde{u} E \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{E}_{0} \right) + \\ + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[ \frac{\partial}{\partial \xi} \left( - \tilde{\rho}_{e} \tilde{u}^{2} (1-\tilde{u})^{2} + 7 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \tilde{u} (1-\tilde{u}) + 3 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} (\tilde{u}-1) - \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \tilde{u}^{2} - 5 \frac{V_{0e}^{4}}{u_{0}^{4}} \frac{\tilde{p}_{e}^{2}}{\tilde{\rho}_{e}} \right) + \\ + E \left( -2 \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{E}_{0} \right) \right] \right\} + \\ 583 \qquad + E \left( -2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1-\tilde{u})) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{E}_{0} \right) \right] \right\} - \\ 583 \qquad + E \left( -2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1-\tilde{u})) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{e} \right) \left( \frac{\partial \tilde{\varphi}}{\partial \xi} - \tilde{U}_{11}' \sin\left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3}\right) - \tilde{E}_{0} \right) -$$

$$-2E^{2}\frac{H}{\tilde{u}^{2}}\tilde{\rho}_{e}\left[\left(-\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}+\tilde{U}_{11}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)+\tilde{E}_{0}\right)^{2}+\frac{1}{2}\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right)^{2}+\frac{3}{2}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right)^{2}+6\left(\tilde{U}_{11}'\right)^{2}+\frac{16}{\pi}\left(\tilde{U}_{10}'\tilde{U}_{11}'\right)\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right]=\\=-\frac{\tilde{u}^{2}}{Hu_{0}^{2}}\left(V_{0e}^{2}\tilde{p}_{e}-V_{0p}^{2}\tilde{p}_{p}\left(1+\frac{m_{p}}{m_{e}}\right)\right)$$
(38)

585

587 Two classes of parameters were used by the mathematical modeling – parameters and scales 588 which were not changed during calculations and varied parameters indicated in Table 4.

589 Parameters, scales and Cauchy conditions which are common for modeling with the external590 field:

591 
$$\frac{m_e}{m_p} = 5 \cdot 10^{-5}$$
, the scales  $\rho_0 = 10^{-10} g/cm^3$ ,  $u_0 = 5 \cdot 10^6 cm/s$ ,  $V_{0e} = 5 \cdot 10^6 cm/s$ ,

592 
$$V_{0p} = 5 \cdot 10^4 \text{ cm/s}$$
,  $x_0 = a = 0.142 \text{ nm}$ ,  $\varphi_0 = 10^{-4} \frac{e}{a} = 3.4 \cdot 10^{-6} \text{ CGSE}_{\varphi}$ .

593 Dimensionless parameters  $R = 3 \cdot 10^{-3}$ , E=0.1, H = 15 (by  $N_R = 1$ ). Admit that for the lattice 594  $U \sim V_{1,(10)} \sim V_{1,(11)} \sim \varphi_0$  and choose  $\tilde{U}'_{10} = 10$ ,  $\tilde{U}'_{11} = 10$ .

595 Cauchy conditions 
$$\tilde{\rho}_e(0)=1$$
,  $\tilde{\rho}_p(0)=2\cdot 10^4$ ,  $\tilde{p}_e(0)=1$ ,  $\tilde{p}_p(0)=2\cdot 10^4$ ,  $\tilde{\varphi}(0)=1$ ,  $\frac{\partial \tilde{\rho}_e}{\partial \tilde{\xi}}(0)=0$ .

- 596  $\frac{\partial \tilde{\rho}_p}{\partial \tilde{\xi}}(0) = 0.$
- 597

Table 4. Varied parameters in calculations with the external electric field.

Variant №	${\widetilde E}_0$	$rac{\partial \widetilde{arphi}}{\partial \widetilde{\xi}}(0)$	${\partial {\widetilde p}_{_p}\over\partial {\widetilde \xi}}(0)$	$rac{\partial {\widetilde p}_e}{\partial {\widetilde \xi}}(0)$
1	0	0	0	0
7.0	10	10	0	0
7.1	10	10	10	-1
8.0	100	100	0	0
8.1	100	100	10	0
9.0	10000	10000	0	0
9.1	10000	10000	10	-1
	Variant № 1 7.0 7.1 8.0 8.1 9.0 9.1	Variant № $\tilde{E}_0$ 1         0           7.0         10           7.1         10           8.0         100           8.1         100           9.0         10000           9.1         10000	Variant $N_{\mathbb{P}}$ $\tilde{E}_{0}$ $\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}}(0)$ 1         0         0           7.0         10         10           7.1         10         10           8.0         100         100           8.1         100         100           9.0         10000         10000	Variant $\mathbb{N}_{\mathbb{P}}$ $\tilde{E}_{0}$ $\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}}(0)$ $\frac{\partial \tilde{p}_{p}}{\partial \tilde{\xi}}(0)$ 1         0         0         0           7.0         10         10         0           7.1         10         10         10           8.0         100         100         0           8.1         100         100         10           9.0         10000         10000         0

600 The external intensity of the electric field is written as  
601 
$$E_0 = \frac{\varphi_0}{x_0} \tilde{E}_0 = 10^{-4} \frac{e}{a^2} \tilde{E}_0 = 238CGSE_E \tilde{E}_0 = 7.14 \cdot 10^6 \frac{V}{m} \tilde{E}_0$$
. It means that even by  $\tilde{E}_0 = 1$  we are

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602 dealing with the rather strong fields. But namely strong external fields can exert the influence on the 603 soliton structures compared with the Coulomb forces in the lattice. For example in [20] the influence of the external electric field in graphene up to  $10^7 - 10^8 V/m$ . The values  $\widetilde{E}_0$  are 604 indicated in Table 4, variants 9.0 and 9.1 respond to the extremely strong external field. 605

606 Table 4 contains in the first line the reminder about the first variant of calculations reflected on figures 2 – 5. These data (in the absence of the external field,  $\tilde{E}_0 = 0$ ) are convenient 607 608 for the following result comparison. The variants of calculations in Table 4 are grouped on principle of the  $\tilde{E}_0$  increasing. In more details: figures 49 – 58 correspond to  $\tilde{E}_0 = 10$ , figures 59 – 68 609 correspond to  $\tilde{E}_0 = 100$ , figures 69 – 80 correspond to  $\tilde{E}_0 = 10000$ . 610

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- Fig. 50. u velocity  $\tilde{u}$ . (Variant 7.0). (solid line); p – the positive particles pressure.
- (Variant 7.0). 616
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- 7232. Figures 75 77 demonstrate the typical situation when the area of possible numerical724calculations for a physical variable does not coincide with area  $\tilde{u} = 1$  where the soliton725regime exists.
- 7263. In the area of the soliton existence the condition  $\tilde{u} = 1$  is fulfilled with the high accuracy727defined practically by accuracy of the choosed numerical method (see Figs. 50, 55, 60, 65,72870, 77).
- 4. As a rule for the choosed topology of the electric field the size of the soliton existence isgrowing with increasing of the electric field intensity.
- 731 5. Under the influence of the external electric field the captured electron cloud is displacing in 732 the opposite direction (of the negative variable  $\tilde{\xi}$ ). The soliton kernel is loosing its 733 symmetry.
- 734
  6. The redistribution of the self-consistent effective charge creates the self-consistence field
  735 with the opposite (to the external field) direction, (see Figs. 53, 58, 63, 68, 73, 80).
- 736 7. The quantum pressure of the positive particle is growing with the  $\tilde{\xi}$  increase. On the whole 737 the specific features of the  $\tilde{p}$ ,  $\tilde{q}$  pressures are defined by the process of the soliton 738 formation.

740

# 741 Conclusion

The origin of the charge density waves (CDW) is a long-standing problem relevant to 742 743 a number of important issues in condensed matter physics. Mathematical modeling of the CDW 744 expansion as well as the problem of the high temperature superconduction can be solved only on the 745 basement of the nonlocal quantum hydrodynamics in particular on the basement of the Alexeev 746 non-local quantum hydrodynamics. It is known that the Schrödinger – Madelung quantum physics 747 leads to the destruction of the wave packets and can not be used for the solution of this kind of 748 problems. The appearance in mathematics the soliton solutions is the rare and remarkable effect. As we see the soliton's appearance in the generalized hydrodynamics created by Alexeev is an 749 750 "ordinary" oft-recurring fact. The realized here mathematical modeling CDW expansion support 751 established in [1, 3] mechanism of the relay ("estafette") motion of the soliton' system ("lattice ion 752 - electron") which is realizing by the absence of chemical bonds. Important to underline that the 753 soliton mechanism of CDW expansion in graphene (and other substances like NbSe<sub>2</sub>) takes place 754 in the extremely large diapason of physical parameters. But CDW existence belongs to effects 755 convoying the high temperature superconductivity. It means that the high temperature 756 superconductivity can be explained in the frame of the non-local soliton quantum hydrodynamics.

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