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	Application of Non-local Quantum
	Hydrodynamics to the Description of the
(Charge Density Waves in the Graphene Crystal
	Lattice.
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st	ructure of solitons on the different physical parameters is investigated. Keywords: The theory of solitons; Generalized hydrodynamic equations; Quantun on-local hydrodynamics; Theory of transport processes in graphene.
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pł Fo st be	We deliver here some main ideas and deductions of the generalized Boltzmann hysical kinetics and non-local physics developed by B. Alexeev (see for example $[1 - 10]$), or simplicity, the fundamental methodic aspects are considered from the qualitative andpoint of view avoiding excessively cumbersome formulas. A rigorous description care found, for example, in the monograph [6]. In 1872 L Boltzmann [11, 12] published his kinetic equation for the one-particle stribution function (DF) $f(\mathbf{r}, \mathbf{v}, t)$. He expressed the equation in the form
	$Df/Dt = J^B(f), \qquad (1.1)$
w	here J^B is the local collision integral, and $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{v}}$ is the substantia
(p re ga in	particle) derivative, \mathbf{v} and \mathbf{r} being the velocity and radius vector of the particle espectively. Boltzmann equation (1.1) governs the transport processes in a one-component as, which is sufficiently rarefied that only binary collisions between particles are of aportance and valid only for two character scales, connected with the hydrodynamic time
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42 scale and the time-scale between particle collisions. While we are not concerned here with 43 the explicit form of the collision integral, note that it should satisfy conservation laws of point-44 like particles in binary collisions. Integrals of the distribution function (i.e. its moments) 45 determine the macroscopic hydrodynamic characteristics of the system, in particular the 46 number density of particles n and the temperature T. The Boltzmann equation (BE) is not 47 of course as simple as its symbolic form above might suggest, and it is in only a few special cases that it is amenable to a solution. One example is that of a maxwellian distribution in a 48 49 locally, thermodynamically equilibrium gas in the event when no external forces are present.

50 In this case the equality $J^B = 0$ and $f = f_0$ is met, giving the maxwellian distribution

51 function f_0 . A weak point of the classical Boltzmann kinetic theory is the way it treats the

dynamic properties of interacting particles. On the one hand, as the so-called "physical" derivation of the BE suggests, Boltzmann particles are treated as material points; on the other hand, the collision integral in the BE brings into existence the cross sections for collisions between particles. A rigorous approach to the derivation of the kinetic equation for f (noted in following as KE_f) is based on the hierarchy of the Bogolyubov-Born-Green-

- 57 Kirkwood-Yvon (BBGKY) [1, 6, 13, 14] equations.
- 58

A KE_{f} obtained by the multi-scale method turns into the BE if one ignores the

change of the distribution function (DF) over a time of the order of the collision time (or, equivalently, over a length of the order of the particle interaction radius). It is important to note [1 - 6] that accounting for the third of the scales mentioned above leads (*prior* to introducing any approximation destined to break the Bogolyubov chain) to additional terms, generally of the same order of magnitude, appear in the BE. If the correlation functions is used to derive KE_f from the BBGKY equations, then the passage to the BE means the neglect of non-local effects.

66 Given the above difficulties of the Boltzmann kinetic theory, the following clearly inter 67 related questions arise. First, what is a physically infinitesimal volume and how does its 68 introduction (and, as the consequence, the unavoidable smoothing out of the DF) affect the 69 kinetic equation? This question can be formulated in (from the first glance) the paradox form 70 - what is the size of the point in the physical system? Second, how does a systematic account for the proper diameter of the particle in the derivation of the KE_{f} affect the 71 72 Boltzmann equation? In the theory developed by B. Alexeev, we refer to the corresponding 73 KE_f as Generalized Boltzmann Equation (GBE). The derivation of the GBE and the 74 applications of GBE are presented, in particular, in monograph [6]. Accordingly, our purpose 75 is first to explain the essence of the physical generalization of the BE.

Let a particle of finite radius be characterized, as before, by the position vector **r** and velocity **v** of its center of mass at some instant of time *t*. Let us introduce physically small volume (**PhSV**) as element of measurement of macroscopic characteristics of physical system for a point containing in this **PhSV**. We should hope that **PhSV** contains sufficient particles N_{ph} for statistical description of the system. In other words, a net of physically small volumes covers the whole investigated physical system.

Every **PhSV** contains entire quantity of point-like Boltzmann particles, and *the same DF* f *is prescribed for whole* **PhSV** *in Boltzmann physical kinetics.* Therefore, Boltzmann particles are fully "packed" in the reference volume. Let us consider two adjoining physically small volumes **PhSV**₁ and **PhSV**₂. We have in principle another situation for the particles of finite size moving in physical small volumes, which are *open* thermodynamic systems.

Then, the situation is possible where, at some instant of time *t*, the particle is located on the interface between two volumes. In so doing, the lead effect is possible (say, for 89 $PhSV_2$), when the center of mass of particle moving to the neighboring volume $PhSV_2$ is 90 still in PhSV₁. However, the delay effect takes place as well, when the center of mass of particle moving to the neighboring volume (say, PhSV₂) is already located in PhSV₂ but a 91

92 part of the particle still belongs to $PhSV_1$.

93 Moreover, even the point-like particles (starting after the last collision near the boundary between two mentioned volumes) can change the distribution functions in the 94 95 neighboring volume. The adjusting of the particles dynamic characteristics for translational degrees of freedom takes several collisions. As result, we have in the definite sense "the 96 97 Knudsen layer" between these volumes. This fact unavoidably leads to fluctuations in mass and hence in other hydrodynamic quantities. Existence of such "Knudsen layers" is not 98 connected with the choice of space nets and fully defined by the reduced description for 99 100 ensemble of particles of finite diameters in the conceptual frame of open physically small 101 volumes, therefore - with the chosen method of measurement.

102 This entire complex of effects defines non-local effects in space and time. The 103 corresponding situation is typical for the theoretical physics - we could remind about the role 104 of probe charge in electrostatics or probe circuit in the physics of magnetic effects.

Suppose that DF f corresponds to **PhSV**₁ and DF $f - \Delta f$ is connected with 105 PhSV₂ for Boltzmann particles. In the boundary area in the first approximation, fluctuations 106 107 will be proportional to the mean free path (or, equivalently, to the mean time between the collisions). Then for PhSV the correction for DF should be introduced as 108

$$f^{a} = f - \tau D f / D t \tag{1.2}$$

in the left hand side of classical BE describing the translation of DF in phase space. As the 110 111 result $Df^{a}/Dt = J^{B}$.

(1.3)

112

where J^{B} is the Boltzmann local collision integral. 113

Important to notice that it is only qualitative explanation of GBE derivation obtained 114 115 earlier (see for example [6]) by different strict methods from the BBGKY – chain of kinetic equations. The structure of the KE_{f} is generally as follows 116

117
$$\frac{Df}{Dt} = J^B + J^{nonlocal}, \qquad (1.4)$$

where $J^{nonlocal}$ is the non-local integral term incorporating the non-local time and space 118 effects. The generalized Boltzmann physical kinetics, in essence, involves a local 119 120 approximation

121
$$J^{nonlocal} = \frac{D}{Dt} \left(\tau \frac{Df}{Dt} \right)$$
(1.5)

122 for the second collision integral, here τ being the mean time *between* the particle collisions. 123 We can draw here an analogy with the Bhatnagar - Gross - Krook (BGK) approximation for J^{B} , 124

125
$$J^B = \frac{f_0 - f}{\tau},$$
 (1.6)

126 which popularity as a means to represent the Boltzmann collision integral is due to the huge 127 simplifications it offers. In other words - the local Boltzmann collision integral admits 128 approximation via the BGK algebraic expression, but more complicated non-local integral 129 can be expressed as differential form (1.5). The ratio of the second to the first term on the

right-hand side of Eq. (1.4) is given to an order of magnitude as $J^{nonlocal}/J^B \approx O(\text{Kn}^2)$ and at large Knudsen numbers (Kn defining as ratio of mean free path of particles to the character hydrodynamic length) these terms become of the same order of magnitude. It would seem that at small Knudsen numbers answering to hydrodynamic description the contribution from the second term on the right-hand side of Eq. (1.4) is negligible.

This is not the case, however. When one goes over to the hydrodynamic approximation (by multiplying the kinetic equation by collision invariants and then integrating over velocities), the Boltzmann integral part vanishes, and the second term on the right-hand side of Eq. (1.4) gives a single-order contribution in the generalized Navier - Stokes description. Mathematically, we cannot neglect a term with a small parameter in front of the higher derivative. Physically, the appearing additional terms are due to viscosity and they

141 correspond to the small-scale Kolmogorov turbulence [6]. The integral term $J^{nonlocal}$ turns 142 out to be important both at small and large Knudsen numbers in the theory of transport 143 processes. Thus, $\tau Df/Dt$ is the distribution function fluctuation, and writing Eq. (1.3) 144 without taking into account Eq. (1.2) makes the BE non-closed. From viewpoint of the 145 fluctuation theory, Boltzmann employed the simplest possible closure procedure $f^a = f$.

Then, the additional GBE terms (as compared to the BE) are significant for any Kn,
and the order of magnitude of the difference between the BE and GBE solutions is
impossible to tell beforehand. For GBE the generalized H-theorem is proven [3, 6].

149 It means that the local Boltzmann equation does not belong even to the class of 150 minimal physical models and corresponds so to speak to "the likelihood models". This remark refers also to all consequences of the Boltzmann kinetic theory including "classical" 152 hydrodynamics.

153 Obviously the generalized hydrodynamic equations (GHE) will explicitly involve 154 fluctuations proportional to τ . In the hydrodynamic approximation, the mean time τ 155 between the collisions is related to the dynamic viscosity μ by

(1.7)

156 $\tau p = \Pi \mu,$

[13, 14]. For example, the continuity equation changes its form and will contain terms
proportional to viscosity. On the other hand, if the reference volume extends over the whole
cavity with the hard walls, then the classical conservation laws should be obeyed, and this is
exactly what the monograph [6] proves. Now several remarks of principal significance:

161 1. All fluctuations are found from the strict kinetic considerations and tabulated [6]. 162 The appearing additional terms in GHE are due to viscosity and they correspond to the 163 small-scale Kolmogorov turbulence. The neglect of formally small terms is equivalent, in 164 particular, to dropping the (small-scale) Kolmogorov turbulence from consideration and is the 165 origin of all principal difficulties in usual turbulent theory. Fluctuations on the wall are equal to zero, from the physical point of view this fact corresponds to the laminar sub-layer. 166 Mathematically it leads to additional boundary conditions for GHE. Major difficulties arose 167 when the question of existence and uniqueness of solutions of the Navier - Stokes equations 168 169 was addressed.

O. A. Ladyzhenskaya has shown for three-dimensional flows that under smooth
initial conditions a unique solution is only possible over a finite time interval. Ladyzhenskaya
even introduced a "correction" into the Navier - Stokes equations in order that its unique
solvability could be proved; GHE do not lead to these difficulties.

174 2. It would appear that in continuum mechanics the idea of discreteness can be 175 abandoned altogether and the medium under study be considered as a continuum in the 176 literal sense of the word. Such an approach is of course possible and indeed leads to the 177 Euler equations in hydrodynamics. However, when the viscosity and thermal conductivity 178 effects are to be included, a totally different situation arises. As is well known, the dynamical 179 viscosity is proportional to the mean time τ between the particle collisions, and a continuum 180 medium in the Euler model with $\tau = 0$ implies that neither viscosity nor thermal conductivity 181 is possible.

182 3. The non-local kinetic effects listed above will always be relevant to a kinetic theory 183 using one particle description – including, in particular, applications to liquids or plasmas, 184 where self-consistent forces with appropriately cut-off radius of their action are introduced to 185 expand the capability of GBE [5, 6]. Fluctuation effects occur in any open thermodynamic 186 system bounded by a control surface transparent to particles. GBE (1.3) leads to generalized 187 hydrodynamic equations [6] as the local approximation of non local effects, for example, to 188 the continuity equation

$$\frac{\partial \rho^a}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0)^a = 0, \qquad (1.8)$$

190 where ρ^a , \mathbf{v}_0^a , $(\rho \mathbf{v}_0)^a$ are calculated in view of non-locality effect in terms of gas density

191 ho, hydrodynamic velocity of flow \mathbf{v}_0 , and density of momentum flux $ho \mathbf{v}_0$; for locally

192 Maxwellian distribution, ρ^a , $(\rho \mathbf{v}_0)^a$ are defined by the relations

193
$$(\rho - \rho^{a})/\tau = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_{0}), \ (\rho \mathbf{v}_{0} - (\rho \mathbf{v}_{0})^{a})/\tau = \frac{\partial}{\partial t} (\rho \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{v}_{0} \mathbf{v}_{0} + \ddot{\mathbf{I}} \cdot \frac{\partial p}{\partial \mathbf{r}} - \rho \mathbf{a},$$
194
$$(1.9)$$

195 where \ddot{I} is a unit tensor, and a is the acceleration due to the effect of mass forces.

196 In the general case, the parameter $\tau \square$ is the non-locality parameter; in quantum 197 hydrodynamics, the "time-energy" uncertainty relation defines its magnitude. Obviously the 198 mentioned non-local effects can be discussed from viewpoint of breaking of the Bell's 199 inequalities [15] because in the non-local theory the measurement (realized in **PhSV**₁) has 200 influence on the measurement realized in the adjoining space-time point in **PhSV**₂ and 201 verse versa.

The violation of Bell's inequalities [15] is found for local statistical theories, and the transition to non-local description is inevitable.

Notice that the application of the above principles also leads to the modification of the system of Maxwell equations. While the traditional formulation of this system does not involve the continuity equation, its derivation explicitly employs the equation

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$$\frac{\partial \rho^a}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{j}^a = 0, \qquad (1.10)$$

where ρ^a is the charge per unit volume, and \mathbf{j}^a is the current density, both calculated without accounting for the fluctuations. As a result, the system of Maxwell equations written in the standard notation, namely

211
$$\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{B} = 0, \ \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{D} = \rho^{a}, \ \frac{\partial}{\partial \mathbf{r}} \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \ \frac{\partial}{\partial \mathbf{r}} \times \mathbf{H} = \mathbf{j}^{a} + \frac{\partial \mathbf{D}}{\partial t}$$
(1.11)

212 contains

213

189

$$\rho^{a} = \rho - \rho^{f^{l}}, \ \mathbf{j}^{a} = \mathbf{j} - \mathbf{j}^{f^{l}}. \tag{1.12}$$

The ρ^{fl} , j^{fl} fluctuations calculated using the generalized Boltzmann equation are given, for example, in Ref. [2, 4, 6].

Now we can turn our attention to the quantum hydrodynamic description of individual particles. The abstract of the classical Madelung's paper [16] contains only one phrase: "It is shown that the Schrödinger equation for one-electron problems can be transformed into the form of hydrodynamic equations".

- The following conclusion of principal significance can be done from the generalized quantum consideration [7, 8]:
- Madelung's quantum hydrodynamics is equivalent to the Schrödinger equation (SE) and leads to description of the quantum particle evolution in the form of Euler equation and continuity equation.
- 225 2. SE is consequence of the Liouville equation as result of the local approximation of 226 non-local equations.
- 2273. Generalized Boltzmann physical kinetics defines the strict approximation of non-228local effects in space and time and after transmission to the local approximation229leads to parameter τ , which on the quantum level corresponds to the uncertainty230principle "time-energy".
- 231 232

4. GHE lead to SE as a deep particular case of the generalized Boltzmann physical kinetics and therefore of non-local hydrodynamics.

In principal GHE needn't in using of the "time-energy" uncertainty relation for estimation of the value of the non-locality parameter τ . Moreover, the "time-energy" uncertainty relation does not lead to the exact relations and from position of non-local physics is only the simplest estimation of the non-local effects.

237 Really, let us consider two neighboring physically infinitely small volumes $PhSV_1$ 238 and $PhSV_2$ in a non-equilibrium system. Obviously the time τ should tend to diminish with 239 increasing of the velocities u of particles invading in the nearest neighboring physically 240 infinitely small volume ($PhSV_1$ or $PhSV_2$):

$$\tau = H/u^n . \tag{1.13}$$

However, the value τ cannot depend on the velocity direction and naturally to tie τ with the particle kinetic energy, then

244 $\tau = \frac{H}{mu^2}$, (1.14)

where *H* is a coefficient of proportionality, which reflects the state of physical system. In the simplest case *H* is equal to Plank constant \hbar and relation (1.14) becomes compatible with the Heisenberg relation.

248 It is known that Ehrenfest adiabatic theorem is one of the most important and widely 249 studied theorems in Schrödinger quantum mechanics. It states that if we have a slowly 250 changing Hamiltonian that depends on time, and the system is prepared in one of the 251 instantaneous eigenstates of the Hamiltonian then the state of the system at any time is 252 given by an the instantaneous eigenfunction of the Hamiltonian up to multiplicative phase 253 factors [17 - 21]. Since the establishment of this theorem many fundamental results have 254 been obtained, such as Landau – Zener transition [17, 18], the Gell-Mann-Low theorem [19], 255 Berry phase [20] and holonomy [21].

The adiabatic theory can be naturally incorporated in generalized quantum hydrodynamics based on local approximations of non-local terms. In the simplest case if ΔQ is the elementary heat quantity delivered for a system executing the transfer from one

state (the corresponding time moment is t_{in}) to the next one (the time moment t_e) then

260
$$\Delta Q = \frac{1}{\tau} 2\delta(\overline{T}\tau), \qquad (1.15)$$

where $\tau = t_e - t_{in}$ and \overline{T} is the average kinetic energy. For adiabatic case Ehrenfest supposes that

$$2\overline{T}\tau = \Omega_1, \Omega_2, \dots \tag{1.16}$$

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where $\Omega_1, \Omega_2, ...$ are adiabatic invariants. Obviously for Plank's oscillator (compare with (1.14))

$$2\overline{T}\tau = nh. \tag{1.17}$$

266

267 *Conclusion*: adiabatic theorem and consequences of this theory deliver the general 268 quantization conditions for non-local quantum hydrodynamics.

269 Non-local physics demonstrates its high efficiency in many fields – from the atom 270 structure problems to cosmology [9, 10].

The possibility of the non local physics application in the theory of superconductivity is investigated in [22 - 24]. It is shown that by the superconducting conditions the relay ("estafette") motion of the soliton' system ("lattice ion – electron") is realizing without creation of the additional chemical bonds. From the position of the quantum hydrodynamics the problem of creation of the high temperature superconductors leads to finding of materials which lattices could realize the soliton' motion without the soliton destruction. These materials should be created using the technology of quantum dots.

278 This paper is directed on investigation of possible applications of the non-local 279 quantum hydrodynamics in the theory of transport processes in graphene including the 280 effects of the charge density waves (CDW). Is known that graphene, a single-atom-thick 281 sheet of graphite, is a new material which combines aspects of semiconductors and metals. 282 For example the mobility, a measure of how well a material conducts electricity, is higher 283 than for other known material at room temperature. In graphene, a resistivity is of about 1.0 284 microOhm-cm (resistivity defined as a specific measure of resistance; the resistance of a 285 piece material is its resistivity times its length and divided by its cross-sectional area). This is 286 about 35 percent less than the resistivity of copper, the lowest resistivity material known at 287 room temperature.

288 Measurements lead to conclusion that the influence of thermal vibrations on the 289 conduction of electrons in graphene is extraordinarily small. From the other side the typical 290 reasoning exists:

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

297 Obviously this point of view leads to the principal elimination of effects of the high 298 temperature superconductivity. From the mentioned point of view the restrictions in mobilities of known semiconductors can be explained as the influence of the thermal vibration of the 299 atoms. The limit to mobility of electrons in graphene is about 200,000 $cm^2/(V \cdot s)$) at room 300 temperature, compared to about 1,400 $cm^2/(V \cdot s)$ in silicon, and 77,000 $cm^2/(V \cdot s)$ in 301 indium antimonide, the highest mobility conventional semiconductor known. The opinion of a 302 303 part of investigators can be formulated as follows: "Other extrinsic sources in today's fairly 304 dirty graphene samples add some extra resistivity to graphene," (see for example [25]) "so 305 the overall resistivity isn't quite as low as copper's at room temperature yet. However, 306 graphene has far fewer electrons than copper, so in graphene the electrical current is carried 307 by only a few electrons moving much faster than the electrons in copper." Mobility 308 determines the speed at which an electronic device (for instance, a field-effect transistor, 309 which forms the basis of modern computer chips) can turn on and off. The very high mobility 310 makes graphene promising for applications in which transistors much switch extremely fast, 311 such as in processing extremely high frequency signals. The low resistivity and extremely 312 thin nature of graphene also promises applications in thin, mechanically tough, electrically 313 conducting, transparent films. Such films are sorely needed in a variety of electronics 314 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 $YBa_2Cu_3O_{6.67}$ ($T_c = 67$ K)) was realized with the scanning tunneling microscope (STM) and other instruments, STMs scan a surface in steps smaller than an atom.

Superconductivity, in which an electric current flows with zero resistance, was first
discovered in metals cooled very close to absolute zero. New materials called cuprates copper oxides "doped" with other atoms -- superconduct as "high" as minus 123 Celsius.
Some conclusions from direct observations [26, 27]:

1. Observations of high-temperature superconductors show an "energy gap" where electronic states are missing. Sometimes this energy gap appears but the material still does not superconduct - a so-called "pseudogap" phase. The pseudogap appears at higher temperatures than any superconductivity, offering the promise of someday developing materials that would superconduct at or near room temperature.

328 2. STM image of a partially doped cuprate superconductor shows regions with an
 329 electronic "pseudogap". As doping increases, pseudogap regions spread and connect,
 330 making the whole sample a superconductor.

331 3. High temperature superconductivity in layered cuprates can develop from an
 332 electronically ordered state called a charge density wave (CDW). The results of observation
 333 can be interpreted as the creation of the "checkerboard pattern" due to the modulation of the

atomic positions in the CuO_2 layers of $YBa_2Cu_3O_{6+x}$ caused by the charge density wave.

4. Application of the method of high-energy X-ray diffraction shows that a CDW develop at zero field in the normal state of superconducting $YBa_2Cu_3O_{6.67}$ ($T_c = 67$ K). Below T_c the application of a magnetic field suppresses superconductivity and enhances the CDW. It means that the high- T_c superconductivity forms from a pre-existing CDW environment.

Important conclusion: high temperature superconductors demonstrate new type of electronic order and modulation of atomic positions. As it was shown in [22, 24] the mentioned above graphene properties can be explained only in the frame of the self-consistent non-local quantum theory (see for example [7, 8]) which leads to appearance of the soliton waves moving in graphene.

344

345 2. GENERALIZED QUANTUM HYDRODYNAMIC EQUATIONS

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347 Strict consideration leads to the following system of the generalized quantum 348 hydrodynamic equations (GHE) [6] written in the dimensional generalized Euler form: 349 Continuity equation for species α :

$$\frac{\partial}{\partial t} \left\{ \rho_{\alpha} - \tau_{\alpha} \left[\frac{\partial \rho_{\alpha}}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0}) \right] \right\} + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \rho_{\alpha} \mathbf{v}_{0} - \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0} \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{$$

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350

and continuity equation for mixture

$$\frac{\partial}{\partial t} \left\{ \rho - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial \rho_{\alpha}}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0}) \right] \right\} + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \rho \mathbf{v}_{0} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0}) + \mathbf{\tilde{I}} \cdot \frac{\partial \rho_{\alpha}}{\partial \mathbf{r}} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} \times \mathbf{B} \right] \right\} = 0.$$
(2.2)

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Momentum equation for species

$$\frac{\partial}{\partial t} \left\{ \rho_{\alpha} \mathbf{v}_{0} - \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial t} \cdot \rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{\partial \rho_{\alpha}}{\partial t} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} \times \mathbf{B} \right] \right\} - \mathbf{F}_{\alpha}^{(1)} \left[\rho_{\alpha} - \tau_{\alpha} \left(\frac{\partial \rho_{\alpha}}{\partial t} + \frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) \right) \right] - \frac{q_{\alpha}}{m_{\alpha}} \left\{ \rho_{\alpha} \mathbf{v}_{0} - \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial t} \cdot \rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{\partial \rho_{\alpha}}{\partial t} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} \times \mathbf{B} \right] \right\} \times \mathbf{B} + \frac{\partial}{\partial t} \cdot \left\{ \rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \rho_{\alpha} \mathbf{I} - \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \rho_{\alpha} \mathbf{I} \right] + \frac{\partial}{\partial t} \cdot \rho_{\alpha} (\mathbf{v}_{0} \mathbf{v}_{0}) \mathbf{v}_{0} + 2 \mathbf{I} \left[\frac{\partial}{\partial t} \cdot (\rho_{\alpha} \mathbf{v}_{0}) \right] + \frac{\partial}{\partial t} \cdot (\mathbf{I} \rho_{\alpha} \mathbf{v}_{0}) - \mathbf{F}_{\alpha}^{(1)} \rho_{\alpha} \mathbf{v}_{0} - \rho_{\alpha} \mathbf{v}_{0} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} [\mathbf{v}_{0} \times \mathbf{B}] \mathbf{v}_{0} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} [\mathbf{v}_{0} \times \mathbf{B}] \right] \right\} = \int m_{\alpha} \mathbf{v}_{\alpha} J_{\alpha}^{s, el} d\mathbf{v}_{\alpha} + \int m_{\alpha} \mathbf{v}_{\alpha} J_{\alpha}^{s, inel} d\mathbf{v}_{\alpha}.$$
(2.3)

Generalized moment equation for mixture

$$\frac{\partial}{\partial t} \left\{ \rho \mathbf{v}_{0} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial t} \cdot \rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{\partial \rho_{\alpha}}{\partial t} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} \times \mathbf{B} \right] \right\} - \sum_{\alpha} \mathbf{F}_{\alpha}^{(1)} \left[\rho_{\alpha} - \tau_{\alpha} \left(\frac{\partial \rho_{\alpha}}{\partial t} + \frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) \right) \right] - \sum_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} \left\{ \rho_{\alpha} \mathbf{v}_{0} - \tau_{\alpha}^{(0)} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial t} \cdot \rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{\partial \rho_{\alpha}}{\partial t} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} \times \mathbf{B} \right] \right\} \times \mathbf{B} + \frac{\partial}{\partial t} \cdot \left\{ \rho \mathbf{v}_{0} \mathbf{v}_{0} + \rho \mathbf{I} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \rho_{\alpha} \mathbf{I} \right] + \frac{\partial}{\partial t} \cdot \rho_{\alpha} (\mathbf{v}_{0} \mathbf{v}_{0}) \mathbf{v}_{0} + 2 \mathbf{I} \left[\frac{\partial}{\partial t} \cdot (\rho_{\alpha} \mathbf{v}_{0}) \right] + \frac{\partial}{\partial t} \cdot \left(\mathbf{I} \rho_{\alpha} \mathbf{v}_{0} \right) - \mathbf{F}_{\alpha}^{(1)} \rho_{\alpha} \mathbf{v}_{0} - \rho_{\alpha} \mathbf{v}_{0} \mathbf{F}_{\alpha}^{(1)} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} [\mathbf{v}_{0} \times \mathbf{B}] \mathbf{v}_{0} - \frac{q_{\alpha}}{m_{\alpha}} \rho_{\alpha} \mathbf{v}_{0} [\mathbf{v}_{0} \times \mathbf{B}] \right\} = 0$$

$$(2.4)$$

364 Energy equation for component

365

$$\frac{\partial}{\partial t} \left\{ \frac{\rho_{\alpha} v_{0}^{2}}{2} + \frac{3}{2} p_{\alpha} + \varepsilon_{\alpha} n_{\alpha} - \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{\rho_{\alpha} v_{0}^{2}}{2} + \frac{3}{2} p_{\alpha} + \varepsilon_{\alpha} n_{\alpha} \right) + \frac{\partial}{\partial t} \cdot \left(\frac{1}{2} \rho_{\alpha} v_{0}^{2} \mathbf{v}_{0} + \frac{5}{2} p_{\alpha} \mathbf{v}_{0} + \varepsilon_{\alpha} n_{\alpha} \mathbf{v}_{0} \right) - \mathbf{F}_{\alpha}^{(1)} \cdot \rho_{\alpha} \mathbf{v}_{0} \right] \right\} + \frac{\partial}{\partial t} \cdot \left\{ \frac{1}{2} \rho_{\alpha} v_{0}^{2} \mathbf{v}_{0} + \frac{5}{2} p_{\alpha} \mathbf{v}_{0} + \varepsilon_{\alpha} n_{\alpha} \mathbf{v}_{0} - \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_{\alpha} v_{0}^{2} \mathbf{v}_{0} + \frac{5}{2} p_{\alpha} \mathbf{v}_{0} + \varepsilon_{\alpha} n_{\alpha} \mathbf{v}_{0} - \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_{\alpha} v_{0}^{2} \mathbf{v}_{0} + \frac{1}{2} p_{\alpha} v_{0}^{2} \mathbf{v}_{0} + \frac{5}{2} p_{\alpha} \mathbf{v}_{0} + \varepsilon_{\alpha} n_{\alpha} \mathbf{v}_{0} \right) + \frac{\partial}{\partial t} \cdot \left(\frac{1}{2} \rho_{\alpha} v_{0}^{2} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{7}{2} p_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{1}{2} p_{\alpha} v_{0}^{2} \mathbf{I} + \frac{5}{2} \frac{p_{\alpha}^{2}}{\rho_{\alpha}} \mathbf{I} + \varepsilon_{\alpha} n_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \varepsilon_{\alpha} \frac{p_{\alpha}}{m_{\alpha}} \mathbf{I} \right) - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} \cdot \mathbf{v}_{0} \mathbf{v}_{0} - p_{\alpha} \mathbf{F}_{\alpha}^{(1)} \cdot \mathbf{I} - \frac{1}{2} \rho_{\alpha} v_{0}^{2} \mathbf{F}_{\alpha}^{(1)} - \frac{3}{2} \mathbf{F}_{\alpha}^{(1)} p_{\alpha} - \frac{\rho_{\alpha} v_{0}^{2}}{2} \frac{q_{\alpha}}{m_{\alpha}} [\mathbf{v}_{0} \times \mathbf{B}] - \frac{5}{2} p_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} [\mathbf{v}_{0} \times \mathbf{B}] - \varepsilon_{\alpha} n_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} [\mathbf{v}_{0} \times \mathbf{B}] - \varepsilon_{\alpha} n_{\alpha} \mathbf{F}_{\alpha}^{(1)} \right] \right\} - \left\{ \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} \cdot \mathbf{v}_{0} - \tau_{\alpha} \left[\mathbf{F}_{\alpha}^{(1)} \cdot \mathbf{F}_{\alpha}^{(1)} \cdot \left(\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_{0}) + \frac{\partial}{\partial t} \cdot \rho_{\alpha} \mathbf{v}_{0} \mathbf{v}_{0} + \frac{\partial}{\partial t} \cdot p_{\alpha} \mathbf{I} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - q_{\alpha} n_{\alpha} [\mathbf{v}_{0} \times \mathbf{B}] \right) \right\} \right\} = (2.5)$$

366

367

368 and after summation the generalized energy equation for mixture

$$\begin{aligned} \frac{\partial}{\partial t} \left\{ \frac{\rho v_0^2}{2} + \frac{3}{2} p + \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{\rho_{\alpha} v_0^2}{2} + \frac{3}{2} p_{\alpha} + \varepsilon_{\alpha} n_{\alpha} \right) + \right. \\ \frac{\partial}{\partial t} \cdot \left(\frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 + \varepsilon_{\alpha} n_{\alpha} \mathbf{v}_0 \right) - \mathbf{F}_{\alpha}^{(1)} \cdot \rho_{\alpha} \mathbf{v}_0 \right] \right\} + \\ \frac{\partial}{\partial t} \cdot \left\{ \frac{1}{2} \rho v_0^2 \mathbf{v}_0 + \frac{5}{2} p \mathbf{v}_0 + \mathbf{v}_0 \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 + \mathbf{v}_0 \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 + \mathbf{v}_0 \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 + \mathbf{v}_0 \sum_{\alpha} \varepsilon_{\alpha} n_{\alpha} - \sum_{\alpha} \tau_{\alpha} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 \mathbf{v}_0 + \frac{1}{2} p_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 \mathbf{v}_0 + \frac{1}{2} p_{\alpha} v_0^2 \mathbf{v}_0 + \frac{5}{2} p_{\alpha} \mathbf{v}_0 \mathbf{v}_0 + \frac{\partial}{\partial t} \cdot \left(\frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{v}_0 \mathbf{v}_0 + \frac{7}{2} p_{\alpha} \mathbf{v}_0 \mathbf{v}_0 + \frac{1}{2} p_{\alpha} v_0^2 \mathbf{v}_0^2 \mathbf{I} + \frac{5}{2} \frac{p_{\alpha}}{\rho_{\alpha}} \mathbf{v}_0 \mathbf{v}_0 + \varepsilon_{\alpha} \frac{p_{\alpha}}{m_{\alpha}} \mathbf{I} \right] - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} \cdot \mathbf{v}_0 \mathbf{v}_0 - p_{\alpha} \mathbf{F}_{\alpha}^{(1)} \cdot \mathbf{I} - \frac{1}{2} \rho_{\alpha} v_0^2 \mathbf{F}_{\alpha}^{(1)} - \frac{3}{2} \mathbf{F}_{\alpha}^{(1)} p_{\alpha} - \frac{\rho_{\alpha} v_0^2}{2} \frac{q_{\alpha}}{m_{\alpha}} [\mathbf{v}_0 \times \mathbf{B}] - \frac{5}{2} p_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} [\mathbf{v}_0 \times \mathbf{B}] - \varepsilon_{\alpha} n_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} [\mathbf{v}_0 \times \mathbf{B}] - \varepsilon_{\alpha} n_{\alpha} \mathbf{F}_{\alpha}^{(1)} \right] \right\} - \mathbf{v}_0 \cdot \sum_{\alpha} \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} + \sum_{\alpha} \tau_{\alpha} \mathbf{F}_{\alpha}^{(1)} \cdot \left[\frac{\partial}{\partial t} (\rho_{\alpha} \mathbf{v}_0) + \frac{\partial}{\partial t} \cdot \rho_{\alpha} \mathbf{v}_0 \mathbf{v}_0 + \frac{\partial}{\partial t} \cdot p_{\alpha} \mathbf{I} - \rho_{\alpha} \mathbf{F}_{\alpha}^{(1)} - q_{\alpha} n_{\alpha} [\mathbf{v}_0 \times \mathbf{B}] \right] = 0.$$

(2.6)

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370 371

387

Here $\mathbf{F}_{\alpha}^{(1)}$ are the forces of the non-magnetic origin, **B** - magnetic induction, $\mathbf{\ddot{I}}$ - unit tensor, q_{α} - charge of the α -component particle, p_{α} - static pressure for α -component, ε_{α} - internal energy for the particles of α - component, \mathbf{v}_0 - hydrodynamic velocity for mixture. For calculations in the self-consistent electro-magnetic field the system of non-local Maxwell equations should be added (see (1.11), (1.12)).

377 It is well known that basic Schrödinger equation (SE) of quantum mechanics firstly 378 was introduced as a quantum mechanical postulate. The obvious next step should be done 379 and was realized by E. Madelung in 1927 – the derivation of special hydrodynamic form of 380 SE after introduction wave function Ψ as

381
$$\Psi(x, y, z, t) = \alpha(x, y, z, t) e^{i\beta(x, y, z, t)}.$$
 (2.7)

Using (2.7) and separating the real and imagine parts of SE one obtains

383
$$\frac{\partial \alpha^2}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\frac{\alpha^2 \hbar}{m} \frac{\partial \beta}{\partial \mathbf{r}}\right) = 0, \qquad (2.8)$$

and Eq. (2.8) immediately transforms in continuity equation if the identifications in the Madelung's notations for density ρ and velocity v

$$\rho = \alpha^2 = \Psi \Psi *, \qquad (2.9)$$

$$\mathbf{v} = \frac{\partial}{\partial \mathbf{r}} \left(\beta \hbar / m\right) \tag{2.10}$$

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introduce in Eq. (2.8). Identification for velocity (2.10) is obvious because for 1D flow

390
$$v = \frac{\partial}{\partial x} (\beta \hbar / m) = \frac{\hbar}{m} \frac{\partial}{\partial x} \left[-\frac{1}{\hbar} (E_k t - px) \right] = \frac{1}{m} \frac{\partial}{\partial x} (px) = v_{\phi}, \quad (2.11)$$

391 where v_{ϕ} is phase velocity. The existence of the condition (2.10) means that the 392 corresponding flow has potential

$$\Phi = \beta \hbar / m \,. \tag{2.12}$$

394 As result two effective hydrodynamic equations take place:

395
$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}) = 0, \qquad (2.13)$$

396
$$\frac{\partial \mathbf{v}}{\partial t} + \frac{1}{2} \frac{\partial}{\partial \mathbf{r}} v^2 = -\frac{1}{m} \frac{\partial}{\partial \mathbf{r}} \left(U - \frac{\hbar^2}{2m} \frac{\Delta \alpha}{\alpha} \right).$$
(2.14)

397 But

393

398
$$\frac{\Delta\alpha}{\alpha} = \frac{\Delta\alpha^2}{2\alpha^2} - \frac{1}{\alpha^2} \left(\frac{\partial\alpha}{\partial\mathbf{r}}\right)^2, \qquad (2.15)$$

and the relation (2.15) transforms (2.14) in particular case of the Euler motion equation

400
$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}})\mathbf{v} = -\frac{1}{m} \frac{\partial}{\partial \mathbf{r}} U^*, \qquad (2.16)$$

401 where introduced the efficient potential

402
$$U^* = U - \frac{\hbar^2}{4m\rho} \left[\Delta \rho - \frac{1}{2\rho} \left(\frac{\partial \rho}{\partial \mathbf{r}} \right)^2 \right].$$
(2.17)

404
$$\frac{\hbar^2}{2m\sqrt{\rho}}\Delta\sqrt{\rho} = \frac{\hbar^2}{4m\rho} \left[\Delta\rho - \frac{1}{2\rho} \left(\frac{\partial\rho}{\partial\mathbf{r}}\right)^2\right].$$
 (2.18)

405 Then

406
$$U^* = U + U_{qu} = U - \frac{\hbar^2}{2m\sqrt{\rho}} \Delta\sqrt{\rho} = U - \frac{\hbar^2}{4m\rho} \left[\Delta\rho - \frac{1}{2\rho} \left(\frac{\partial\rho}{\partial\mathbf{r}}\right)^2 \right]. \quad (2.19)$$

407 Some remarks:

- 408 a) SE transforms in hydrodynamic form without additional assumptions. But numerical methods of hydrodynamics are very good developed. As result at the end of seventieth of the last century we realized the systematic calculations of quantum problems using quantum hydrodynamics (see for example [1, 28].
- b) SE reduces to the system of continuity equation and particular case of the Euler equation with the additional potential proportional to \hbar^2 . The physical sense and the
- 414 origin of the Bohm potential are established later in [7, 8, 29].
- c) SE (obtained in the frame of the theory of classical complex variables) cannot contain
 the energy equation in principle. As result in many cases the palliative approach is used
 when for solution of dissipative quantum problems the classical hydrodynamics is used
 with insertion of additional Bohm potential in the system of hydrodynamic equations.
- 419 d) The system of the generalized quantum hydrodynamic equations contains energy 420 equation written for unknown dependent value which can be specified as quantum 421 pressure p_{α} of non-local origin.

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422 The transport properties in graphene can be described at low energies by a 423 massless Dirac-fermion model with chiral guasiparticles [30, 31]. The Boltzmann and 424 Schrödinger approaches are used also [32], [33]. Applications of these approaches are 425 directed on the calculation of kinetic coefficients. The non-local kinetic equations also are used by the authors of this article for calculation of graphene electrical conductivity [34]. 426 427 Here we intend to investigate the possibilities of non-local quantum hydrodynamics for 428 modeling of the charge density waves in grafene. In non-local quantum hydrodynamics the 429 many particles correlations manifest itself in equations in the terms proportional to non-430 locality parameter au.

431 The influence of spin and magnetic moment of particles can be taken into account 432 by the natural elegant way via the internal energy of particles. Really for example electron 433 has the internal energy \mathcal{E}

$$\mathcal{E} = \mathcal{E}_{el \ sn} + \mathcal{E}_{el \ m} \,, \tag{2.20}$$

435 containing the spin and magnetic parts, namely

436

434

437

$$\varepsilon_{el,sp} = \hbar \omega / 2$$
, $\varepsilon_{el,m} = -\mathbf{p}_{\mathbf{m}} \cdot \mathbf{B}$; (2.21)

438 $\mathbf{p}_{\mathbf{m}}$ - electron magnetic moment, \mathbf{B} - magnetic induction. But $p_m = -\frac{e}{m_e}\frac{\hbar}{2c}$, then

439
$$\varepsilon_{el} = \frac{\hbar}{2}\omega_{eff}$$
. Relation (2.20) can be written as

$$\varepsilon = \frac{\hbar}{2} \left[\omega \pm \frac{e}{m_e c} B \right], \tag{2.22}$$

if **B** is directed along the spin direction. On this stage of investigations we omit the influence
of the internal energy of particles, therefore spin waves will be investigated separately.

444

440

4453. GENERALIZED QUANTUM HYDRODYNAMIC EQUATIONS DESCRIBING THE446SOLITON MOVEMENT IN THE CRYSTAL LATTICE

447

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

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

The effective charge is created due to interference of the induced electron waves and correlating potentials as result of the polarized modulation of atomic positions. Therefore in this approach the conduction in graphene convoys the transfer of the positive $(+e, m_p)$ and negative $(-e, m_e)$ 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 and non-potential origin. It was shown [22 24] that mentioned soliton can exist without a chemical bond formation. First of all for better understanding of the
- 462 situation let us investigate the situation for the case when the external forces are absent.
- 463 Introduce the coordinate system ($\xi = x Ct$) moving along the positive direction of the x
- 464 axis with the velocity $C = u_0$, which is equal to the phase velocity of this quantum object.

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465 Let us find the soliton type solutions for the system of the generalized quantum equations for two species mixture. The graphene crystal lattice is 2D flat structure which is 466 considered in the moving coordinate system ($\xi = x - u_0 t$, y). In the following we intend 467 (without taking into account the component's internal energy) to apply generalized non-local 468 469 quantum hydrodynamic equations (2.1) - (2.6) to the investigation of the charge density 470 waves (CDW) in the frame of two species model which lied to the following dimensional 471 equations [6, 8]:

472 Poisson equation for the self-consistent electric field:

$$473 \qquad \frac{\partial^2 \varphi}{\partial \xi^2} + \frac{\partial^2 \varphi}{\partial y^2} = -4\pi e \left\{ \left[n_p - \tau_p \frac{\partial}{\partial \xi} \left(n_p \left(u - u_0 \right) \right) \right] - \left[n_e - \tau_e \frac{\partial}{\partial \xi} \left(n_e \left(u - u_0 \right) \right) \right] \right\}$$
(3.1)

Continuity equation for the positive particles: 474

$$\frac{\partial}{\partial\xi} \left[\rho_{p}(u_{0}-u) \right] + \frac{\partial}{\partial\xi} \left\{ \tau_{p} \frac{\partial}{\partial\xi} \left[\rho_{p}(u-u_{0})^{2} \right] \right\} + \frac{\partial}{\partial\xi} \left\{ \tau_{p} \left[\frac{\partial}{\partial\xi} p_{p} - \rho_{p} F_{p\xi} \right] \right\} + \frac{\partial}{\partialy} \left\{ \tau_{p} \left[\frac{\partial}{\partialy} p_{p} - \rho_{p} F_{py} \right] \right\} = 0$$

$$476 \quad \text{Continuity equation for electrons:}$$

$$(3.2)$$

 $\frac{\partial}{\partial \xi} [\rho_e(u_0 - u)] + \frac{\partial}{\partial \xi} \left\{ \tau_e \frac{\partial}{\partial \xi} [\rho_e(u - u_0)^2] \right\} +$ (3.3) $\frac{\partial}{\partial\xi} \left\{ \tau_e \left[\frac{\partial}{\partial\xi} p_e - \rho_e F_{e\xi} \right] \right\} + \frac{\partial}{\partial y} \left\{ \tau_e \left[\frac{\partial}{\partial y} p_e - \rho_e F_{ey} \right] \right\} = 0$

$$\frac{\partial}{\partial \xi} \{ \rho u (u - u_0) + p \} - \rho_p F_{p\xi} - \rho_e F_{e\xi} +$$

47

$$\frac{\partial \xi}{\partial \xi} \left\{ \tau_{p} \left[\frac{\partial}{\partial \xi} \left\{ 2p_{p}(u_{0} - u) - \rho_{p}u(u_{0} - u)^{2} \right) - \rho_{p}F_{p\xi}(u_{0} - u) \right] \right\} + \frac{\partial}{\partial \xi} \left\{ \tau_{e} \left[\frac{\partial}{\partial \xi} \left\{ 2p_{e}(u_{0} - u) - \rho_{e}u(u_{0} - u)^{2} \right) - \rho_{e}F_{e\xi}(u_{0} - u) \right] \right\} + \frac{\partial}{\partial \xi} \left\{ \tau_{e} \left[\frac{\partial}{\partial \xi} \left(2p_{e}(u_{0} - u) - \rho_{e}u(u_{0} - u)^{2} \right) - \rho_{e}F_{e\xi}(u_{0} - u) \right] \right\} + \frac{\partial}{\partial \xi} \left\{ \tau_{p}F_{p\xi} \left(\frac{\partial}{\partial \xi} \left(\rho_{p}(u - u_{0}) \right) \right) + \tau_{e}F_{e\xi} \left(\frac{\partial}{\partial \xi} \left(\rho_{e}(u - u_{0}) \right) \right) - \frac{\partial}{\partial \xi} \left\{ \tau_{p} \frac{\partial}{\partial \xi} \left\{ p_{p}u \right\} - \frac{\partial}{\partial \xi} \left\{ \tau_{e} \frac{\partial}{\partial \xi} \left(p_{e}u \right) \right\} - \frac{\partial}{\partial \xi} \left\{ \tau_{e} \frac{\partial}{\partial \xi} \left(p_{e}u \right) \right\} + \frac{\partial}{\partial \xi} \left\{ \tau_{e} \left[F_{e\xi} \rho_{e}u \right] \right\} + \frac{\partial}{\partial y} \left\{ \tau_{p} \left[F_{py} \rho_{p}u \right] \right\} + \frac{\partial}{\partial y} \left\{ \tau_{e} \left[F_{ey} \rho_{e}u \right] \right\} = 0 \quad (3.4)$$

482

483

484 Energy equation for the positive particles:

485

$$\frac{\partial}{\partial\xi} \left[\rho_{p} u^{2} (u - u_{0}) + 5 p_{p} u - 3 p_{p} u_{0} \right] - 2 \rho_{p} F_{p\xi} u + \frac{\partial}{\partial\xi} \left\{ \tau_{p} \left[\frac{\partial}{\partial\xi} \left(- \rho_{p} u^{2} (u_{0} - u)^{2} + 7 p_{p} u (u_{0} - u) + 3 p_{p} u_{0} (u - u_{0}) - p_{p} u^{2} - 5 \frac{p_{p}^{2}}{\rho_{p}} \right) - \right] \right\} - \frac{\partial}{\partial\xi} \left\{ \tau_{p} \left[\frac{\partial}{\partial\xi} \left(p_{p} u^{2} + 5 \frac{p_{p}^{2}}{\rho_{p}} \right) - \rho_{p} F_{py} u^{2} - 5 p_{p} F_{py} \right] \right\} - \frac{\partial}{\partial\xi} \left\{ \tau_{p} \left[\frac{\partial}{\partial\xi} \left(\rho_{p} u (u_{0} - u) \right) \right] - 2 \tau_{p} \rho_{p} \left[(F_{p\xi})^{2} + (F_{py})^{2} \right] + \frac{2 \tau_{p} F_{p\xi}}{\rho_{p\xi}} \left[\frac{\partial}{\partial\xi} p_{p} \right] + 2 \tau_{p} F_{py} \left[\frac{\partial}{\partialy} p_{p} \right] = - \frac{p_{p} - p_{e}}{\tau_{ep}} \right] \right\}$$
(3.5)

489 Energy equation for electrons:

490

$$\frac{\partial}{\partial\xi} \left[\rho_{e} u^{2} (u - u_{0}) + 5p_{e} u - 3p_{e} u_{0} \right] - 2\rho_{e} F_{e\xi} u + \\ \frac{\partial}{\partial\xi} \left\{ \tau_{e} \left[\frac{\partial}{\partial\xi} \left(-\rho_{e} u^{2} (u_{0} - u)^{2} + 7p_{e} u (u_{0} - u) + 3p_{e} u_{0} (u - u_{0}) - p_{e} u^{2} - 5\frac{p_{e}^{2}}{\rho_{e}} \right) - \right] \right\} - \\ \frac{\partial}{\partial\xi} \left\{ \tau_{e} \left[\frac{\partial}{\partial\xi} \left(p_{e} u^{2} + 5\frac{p_{e}^{2}}{\rho_{e}} \right) - \rho_{e} F_{ey} u^{2} - 5p_{e} F_{ey} \right] \right\} - \\ \frac{\partial}{\partial\xi} \left\{ \tau_{e} \left[\frac{\partial}{\partial\xi} \left(\rho_{e} u (u_{0} - u) \right) \right] - 2\tau_{e} \rho_{e} \left[(F_{e\xi})^{2} + (F_{ey})^{2} \right] + \\ 2\tau_{e} F_{e\xi} \left[\frac{\partial}{\partial\xi} \rho_{e} \right] + 2\tau_{e} F_{ey} \left[\frac{\partial}{\partialy} \rho_{e} \right] = -\frac{p_{e} - p_{p}}{\tau_{ep}}$$

49

$$\frac{\partial}{\partial y} \left\{ \tau_{e} \left[\frac{\partial}{\partial y} \left(p_{e}u^{2} + 5\frac{p_{e}}{\rho_{e}} \right) - \rho_{e}F_{ey}u^{2} - 5p_{e}F_{ey} \right] \right\} - 2\tau_{e}F_{e\xi} \left[\frac{\partial}{\partial \xi} \left(\rho_{e}u(u_{0} - u) \right) \right] - 2\tau_{e}\rho_{e} \left[\left(F_{e\xi}\right)^{2} + \left(F_{ey}\right)^{2} \right] + 2\tau_{e}F_{e\xi} \left[\frac{\partial}{\partial \xi} p_{e} \right] + 2\tau_{e}F_{ey} \left[\frac{\partial}{\partial y} p_{e} \right] = -\frac{p_{e} - p_{p}}{\tau_{ep}}$$

$$(3.6)$$

49

Here u - hydrodynamic velocity; arphi - self-consistent electric potential; $ho_{_{e}}$, $ho_{_{p}}$ - densities 493 for the electron and positive species; $p_{\scriptscriptstyle e}, \ p_{\scriptscriptstyle p}$ - quantum electron pressure and the pressure 494 of positive species; F_e , F_p - the forces acting on the mass unit of electrons and the positive 495 particles. 496

497 The right hand sides of the energy equations are written in the relaxation forms 498 following from BGK kinetic approximation 499

Non-local parameters can be written in the form (see (1.14))

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500
$$au_{p} = \frac{N_{R}\hbar}{m_{p}u^{2}}, au_{e} = \frac{N_{R}\hbar}{m_{e}u^{2}}, au_{ep} = \frac{1}{\tau_{e}} + \frac{1}{\tau_{p}}$$
 (3.7)

where N_R - integer. 501

502

Acting forces are the sum of three terms: the self-consistent potential force (scalar 503 504 potential φ), connected with the displacement of positive and negative charges, potential 505 forces originated by the graphene crystal lattice (potential U) and the external electrical field creating the intensity E. As result the following relations are valid 506 507

508
$$F_{p\xi} = \frac{e}{m_p} \left(-\frac{\partial \varphi}{\partial \xi} - \frac{\partial U}{\partial \xi} + E_{0\xi} \right), \quad F_{e\xi} = \frac{e}{m_e} \left(\frac{\partial \varphi}{\partial \xi} + \frac{\partial U}{\partial \xi} - E_{0\xi} \right),$$

509

510
$$F_{py} = \frac{e}{m_p} \left(-\frac{\partial \varphi}{\partial y} - \frac{\partial U}{\partial y} + E_{0y} \right), \quad F_{ey} = \frac{e}{m_e} \left(\frac{\partial \varphi}{\partial y} + \frac{\partial U}{\partial y} - E_{0y} \right).$$
(3.8)

511 Let write down these equations in the dimensionless form, where dimensionless 512 symbols are marked by tildes; introduce the scales:

513
$$u = u_0 \widetilde{u}, \quad \xi = x_0 \widetilde{\xi}, \quad y = x_0 \widetilde{y}, \quad \varphi = \varphi_0 \widetilde{\varphi}, \quad \rho_e = \rho_0 \widetilde{\rho}_e, \quad \rho_p = \rho_0 \widetilde{\rho}_p,$$

514 where $u_0, x_0, \varphi_0, \rho_0$ - scales for velocity, distance, potential and density. Let there be 515 also

516
$$p_p = \rho_0 V_{0p}^2 \tilde{p}_p$$
, $p_e = \rho_0 V_{0e}^2 \tilde{p}_e$, where V_{0p} is V_{0e} - the scales for thermal velocities for the

electron and positive species; $F_p = \tilde{F}_p \frac{e\varphi_0}{m_p x_0}$, $F_e = \tilde{F}_e \frac{e\varphi_0}{m_e x_0}$; $\tau_p = \frac{m_e x_0 H}{m_p u_0 \tilde{u}^2}$, 517

 $\tau_e = \frac{x_0 H}{u_0 \tilde{u}^2}$, where dimensionless parameter $H = \frac{N_R \hbar}{m_e x_0 u_0}$ is introduced. Then 518

 $\frac{1}{\tau_{ep}} = \frac{u_0}{x_0} \frac{\tilde{u}^2}{H} \left(1 + \frac{m_p}{m_e}\right).$ 519 520

Let us introduce also the following dimensionless parameters

521
$$R = \frac{e\rho_0 x_0^2}{m_e \varphi_0}, \ E = \frac{e\varphi_0}{m_e u_0^2}.$$
 (3.9)

Taking into account the introduced values the following system of dimensionless 522 non-local hydrodynamic equations for the 2D soliton description can be written: 523 524 Poisson equation for the self-consistent electric field:

525
$$\frac{\partial^2 \tilde{\varphi}}{\partial \tilde{\xi}^2} + \frac{\partial^2 \tilde{\varphi}}{\partial \tilde{y}^2} = -4\pi R \left\{ \frac{m_e}{m_p} \left[\tilde{\rho}_p - \frac{m_e H}{m_p \tilde{u}^2} \frac{\partial}{\partial \tilde{\xi}} (\tilde{\rho}_p (\tilde{u} - 1)) \right] - \left[\tilde{\rho}_e - \frac{H}{\tilde{u}^2} \frac{\partial}{\partial \tilde{\xi}} (\tilde{\rho}_e (\tilde{u} - 1)) \right] \right\}.$$
526 (3.10)

526

527 Continuity equation for the positive particles:

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$$\frac{\partial}{\partial \xi} \left[\tilde{\rho}_{p} \left(1 - \tilde{u} \right) \right] + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} \left[\tilde{\rho}_{p} \left(\tilde{u} - 1 \right)^{2} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} E \tilde{\rho}_{p} \tilde{F}_{p\xi} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} E \tilde{\rho}_{p} \tilde{F}_{p\xi} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} E \tilde{\rho}_{p} \tilde{F}_{py} \right] \right\} = 0$$
(3.11)
ontinuity equation for electrons:

$$\frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{e} (1 - \tilde{u}) \right] + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{e} (\tilde{u} - 1)^{2} \right] \right\} + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{e} - \tilde{\rho}_{e} E \tilde{F}_{e\xi} \right] \right\} + \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{y}} \tilde{p}_{e} - \tilde{\rho}_{e} E \tilde{F}_{ey} \right] \right\} = 0$$
(3.12)

$$\begin{aligned} & \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 \tilde{F}_{p\xi} - \tilde{\rho}_{e} E \tilde{F}_{e\xi} + \\ & \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(2 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} (1 - \tilde{u}) - \tilde{\rho}_{p} \tilde{u} (1 - \tilde{u})^{2} \right) - \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \tilde{F}_{p\xi} (1 - \tilde{u}) \right] \right\} + \\ & \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(2 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} (1 - \tilde{u}) - \tilde{\rho}_{e} \tilde{u} (1 - \tilde{u})^{2} \right) - \tilde{\rho}_{e} E \tilde{F}_{e\xi} (1 - \tilde{u}) \right] \right\} + \\ & \frac{H}{\tilde{u}^{2}} E \left(\frac{m_{e}}{m_{p}} \right)^{2} \tilde{F}_{p\xi} \left(\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} (\tilde{u} - 1) \right) \right) + \frac{H}{\tilde{u}^{2}} E \tilde{F}_{e\xi} \left(\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{e} (\tilde{u} - 1) \right) \right) - \\ & 535 \quad \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left(\tilde{p}_{p} \tilde{u} \right) \right\} - \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{e} \tilde{u} \right) \right\} - \\ & 536 \quad \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{y}} \left(\tilde{p}_{p} \tilde{u} \right) \right\} - \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{y}} \left(\tilde{p}_{e} \tilde{u} \right) \right\} + \end{aligned}$$

537
$$\left(\frac{m_e}{m_p}\right)^2 \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{p\xi} \tilde{\rho}_p \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\rho}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\mu}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\mu}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\mu}_e \tilde{u}] \right\} + \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} E[\tilde{F}_{e\xi} \tilde{\mu}_e \tilde{\mu}] \right\} + \frac{\partial}{\partial$$

538
$$\left(\frac{m_e}{m_p}\right)^2 \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^2} E\left[\tilde{F}_{py} \tilde{\rho}_p \tilde{u}\right] \right\} + \frac{\partial}{\partial \tilde{y}} \left\{ \frac{H}{\tilde{u}^2} E\left[\tilde{F}_{ey} \tilde{\rho}_e \tilde{u}\right] \right\} = 0$$
(3.13)

Energy equation for the positive particles:

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

$$(3.14)$$

542 543 E

541

Energy equation for electrons:

$$\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} E \tilde{F}_{e\xi} \tilde{u} + \frac{\partial}{\partial \xi} \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} - \frac{\partial}{u_{0}^{2}} \right] \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} E \tilde{F}_{e\xi} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} E \tilde{F}_{e\xi} \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} E \tilde{F}_{e\xi} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} E \tilde{F}_{e\xi} \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} E \tilde{F}_{e\xi} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} E \tilde{F}_{e\xi} \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} E \tilde{F}_{e\xi} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} E \tilde{F}_{e\xi} \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} E \tilde{F}_{e\xi} + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} E \tilde{F}_{e\xi} \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u} (1-\tilde{u}) + \tilde{\rho}_{e} \tilde{u}^{2} E \tilde{F}_{e\xi} \tilde{\mu}_{e}^{2} \tilde{p}_{e} E \tilde{F}_{e\xi} \tilde{\rho}_{e}^{2} \tilde{p}_{e} \tilde{E} \tilde{F}_{e\xi} \right] - 2 \tilde{E} \tilde{F}_{e\xi} \tilde{\rho}_{e} \tilde{u}^{2} + 5 \frac{V_{0e}^{4}}{u_{0}^{4}} \tilde{\rho}_{e}^{2} - \tilde{\rho}_{e} \tilde{E} \tilde{F}_{ey} \tilde{u}^{2} - 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} E \tilde{F}_{e\xi} \tilde{F}_{e\xi} \tilde{F}_{e\xi} \tilde{F}_{e\xi} \tilde{F}_{e\xi} \left[\frac{\partial}{\partial \xi} (\tilde{\rho}_{e} \tilde{u} (1-\tilde{u})) \right] - 2 \frac{H}{\tilde{u}^{2}} \tilde{\rho}_{e} E^{2} \left[(\tilde{F}_{e\xi})^{2} + (\tilde{F}_{ey})^{2} \right] + 2 \frac{H}{\tilde{u}^{2}} \tilde{\rho}_{e} \tilde{F}_{ey} \left[\frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial y} \tilde{\rho}_{e} \right] = - \frac{\tilde{u}^{2}}{H u_{0}^{2}} (V_{0e}^{2} \tilde{\rho}_{e} - V_{0p}^{2} \tilde{\rho}_{e}) \left(1 + \frac{m_{p}}{m_{e}} \right)$$
(3.1)

544 545

(3.15)

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546 We have the following dimensionless relations for forces:

547
$$\widetilde{\mathbf{F}}_{\mathbf{p}\xi} = -\frac{\partial \widetilde{\varphi}}{\partial \widetilde{\xi}} - \frac{\partial U}{\partial \widetilde{\xi}} + \widetilde{E}_{\xi}, \quad \widetilde{\mathbf{F}}_{\mathbf{e}\xi} = \frac{\partial \widetilde{\varphi}}{\partial \widetilde{\xi}} + \frac{\partial U}{\partial \widetilde{\xi}} - \widetilde{E}_{\xi},$$

$$\widetilde{\mathbf{F}}_{\mathrm{py}} = -\frac{\partial \widetilde{\varphi}}{\partial \widetilde{y}} - \frac{\partial \widetilde{U}}{\partial \widetilde{y}} + \widetilde{E}_{y}, \qquad \widetilde{\mathbf{F}}_{\mathrm{ey}} = \frac{\partial \widetilde{\varphi}}{\partial \widetilde{y}} + \frac{\partial \widetilde{U}}{\partial \widetilde{y}} - \widetilde{E}_{y}.$$
(3.16)

548 549

- 550 Graphene is a single layer of carbon atoms densely packed in a honeycomb lattice. Figure 1
- reflects the structure of graphene as the 2D hexagonal carbon crystal, the distance a
- between the nearest atoms is equal to $a = 0.142 \ nm$.



553 554 555

Figure 1. Orystal graphene lattice.

556 Elementary cell contains two atoms (for example A and B, figure 1) and the primitive 557 lattice vectors are given by

558
$$\mathbf{a}_1 = \frac{a}{2} (3; \sqrt{3}), \ \mathbf{a}_2 = \frac{a}{2} (3; -\sqrt{3}).$$

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

560
$$\mathbf{\delta}_1 = \frac{a}{2}(1;\sqrt{3}), \ \mathbf{\delta}_2 = \frac{a}{2}(1;-\sqrt{3}), \ \mathbf{\delta}_3 = -a(1;0).$$

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

562
$$\boldsymbol{\delta}_1' = \pm \mathbf{a}_1, \ \boldsymbol{\delta}_2' = \pm \mathbf{a}_2, \ \boldsymbol{\delta}_3' = \pm (\mathbf{a}_2 - \mathbf{a}_1).$$

Let us take the first atom of the elementary cell in the origin of the coordinate system (figure 1) and compose the radii-vector of the second atom with respect to the basis \mathbf{a}_1 μ 565 \mathbf{a}_2 :

566
$$\mathbf{r}_{1} = u\mathbf{a}_{1} + v\mathbf{a}_{2} = u\left(3\frac{a}{2}\mathbf{e}_{x} + \sqrt{3}\frac{a}{2}\mathbf{e}_{y}\right) + v\left(3\frac{a}{2}\mathbf{e}_{x} - \sqrt{3}\frac{a}{2}\mathbf{e}_{y}\right). \quad (3.17)$$

567 Let us find *u* и *v*, taking into account that

568
$$\mathbf{r}_{1} = \mathbf{\delta}_{1} = \frac{a}{2} \left(\mathbf{l}; \sqrt{3} \right) = \frac{a}{2} \mathbf{e}_{x} + \frac{a}{2} \sqrt{3} \mathbf{e}_{y} \,. \tag{3.18}$$

569 Equalizing (3.17) v (3.18), we have $u = \frac{2}{3}$, $v = -\frac{1}{3}$, then

$$\mathbf{r}_1 = \frac{2}{3}\mathbf{a}_1 - \frac{1}{3}\mathbf{a}_2$$
. (3.19)

571 Assume that $V_1(\mathbf{r})$ is the periodical potential created by one sublattice. Then 572 potential of crystal is

$$V(\mathbf{r}) = V_1(\mathbf{r}) + V_1(\mathbf{r} - \mathbf{r}_1) = \sum_{n=0}^{1} V_1(\mathbf{r} - \mathbf{r}_n). \qquad (3.20)$$

574 Atoms in crystal form the periodic structure and as the consequence the corresponding 575 potential is periodic function

$$V_1(\mathbf{r}) = V_1(\mathbf{r} + \mathbf{a}_m)$$

577 where for 2D structure

 $\mathbf{a}_m = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2,$

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

581
$$V_1(\mathbf{r} - \mathbf{r}_n) = \sum_{\mathbf{b}} V_{\mathbf{b}} e^{i\mathbf{b}\cdot(\mathbf{r} - \mathbf{r}_n)}.$$
 (3.21)

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

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

584 \mathbf{b}_1 и \mathbf{b}_2 are the translational vectors of the reciprocal lattice. For graphene

585
586
$$\mathbf{b}_1 = \frac{2\pi}{3a} (1; \sqrt{3}), \quad \mathbf{b}_2 = \frac{2\pi}{3a} (1; -\sqrt{3}).$$
 (3.22)

587 Then

570

573

576

588
$$V(\mathbf{r}) = \sum_{\mathbf{b}} \sum_{n=0}^{1} V_{1\mathbf{b}} e^{i\mathbf{b}\cdot(\mathbf{r}-\mathbf{r}_n)} = \sum_{\mathbf{b}} V_{\mathbf{b}} e^{i\mathbf{b}\cdot\mathbf{r}} , \qquad (3.23)$$

589 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:

590
$$S_{\mathbf{b}} = e^{-i\mathbf{b}\cdot\mathbf{0}} + e^{-i\mathbf{b}\cdot\left(\frac{2}{3}\mathbf{a}_{1} - \frac{1}{3}\mathbf{a}_{2}\right)} = 1 + e^{i\frac{2\pi}{3}(g_{2} - 2g_{1})}.$$
 (3.24)

591

592
$$V(\mathbf{r}) = \sum_{g_1, g_2} V_{1g_1, g_2} e^{i(g_1 \mathbf{b}_1 + g_2 \mathbf{b}_2) \cdot \mathbf{r}} \left(1 + e^{i\frac{2\pi}{3}(g_2 - 2g_1)} \right).$$
(3.25)

593

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

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

597
$$2V_{1,(11)}\left(\cos((\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}) + \cos\left((\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r} - \frac{2\pi}{3}\right) + 2\cos((\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r})\right) - (2\pi)$$

598
$$4V_{1,(20)}\cos((\mathbf{b}_2-\mathbf{b}_1)\cdot\mathbf{r})\cos((\mathbf{b}_2+\mathbf{b}_1)\cdot\mathbf{r}+\frac{2\pi}{3})+$$

599
$$2V_{1,(12)} \left(2\cos((\mathbf{b}_1 + 2\mathbf{b}_2) \cdot \mathbf{r}) + 2\cos((2\mathbf{b}_1 + \mathbf{b}_2) \cdot \mathbf{r}) + \left((\mathbf{a}_1 - \mathbf{a}_2) - \frac{\pi}{2\pi} \right) \right)$$

600
$$\cos\left((\mathbf{b}_1 - 2\mathbf{b}_2) \cdot \mathbf{r} - \frac{\pi}{3}\right) - \cos\left((2\mathbf{b}_1 - \mathbf{b}_2) \cdot \mathbf{r} - \frac{2\pi}{3}\right)\right) +$$

601
$$2V_{1,(22)}\left(2\cos\left(2(\mathbf{b}_1-\mathbf{b}_2)\cdot\mathbf{r}\right)-\cos\left(2(\mathbf{b}_1+\mathbf{b}_2)\cdot\mathbf{r}-\frac{2\pi}{3}\right)\right).$$
(3.26)

602 Using the vectors \mathbf{b}_1 and \mathbf{b}_2 of the reciprocal lattice from (3.22) and coordinates x and y 603 one obtains from (3.26):

604
$$V(x, y) = 2V_{1,(00)} + 4V_{1,(10)}\cos\left(\frac{2\pi}{3a}x + \frac{\pi}{3}\right)\cos\left(\frac{2\pi}{3a}\sqrt{3}y\right) + 605 \qquad 2V = \left(\cos\left(\frac{4\pi}{3a}x - \frac{\pi}{3}\right) + 2\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\right) - 4V = \cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x + \frac{2\pi}{3a}\right)$$

$$605 \qquad 2V_{1,(11)}\left(\cos\left(\frac{4\pi}{3a}x - \frac{\pi}{3}\right) + 2\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\right) - 4V_{1,(20)}\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x + \frac{2\pi}{3}\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x + \frac{2\pi}{3}\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x + \frac{2\pi}{3}\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x + \frac{2\pi}{3}\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}x + \frac{2\pi}{3}\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right) + (11)\cos\left(\frac{4\pi}{3a}\sqrt{3}y\right)\cos\left(\frac{4\pi}{3a}\sqrt{3$$

606
$$4V_{1,(12)}\left(2\cos\left(\frac{2\pi}{a}x\right)\cos\left(\frac{2\pi}{3a}\sqrt{3}y\right) - \sin\left(\frac{2\pi}{3a}x - \frac{\pi}{6}\right)\cos\left(\frac{2\pi}{a}\sqrt{3}y\right)\right) +$$

607
$$2V_{1,(22)}\left(2\cos\left(\frac{8\pi}{3a}\sqrt{3}y\right) - \cos\left(\frac{8\pi}{3a}x - \frac{2\pi}{3}\right)\right).$$
 (3.27)

$$609 \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) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}}{\partial \tilde{\xi}} = \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{\partial \tilde{U}_{10}' \sin\left(\frac{\pi}{3\tilde{a}}\tilde{x} - \frac{\pi}{3}\right) - \frac{$$

610
$$\tilde{U}_{20}' \cos\left(\frac{4\pi}{3\tilde{a}}\sqrt{3}y\right) \sin\left(\frac{4\pi}{3\tilde{a}}x + \frac{2\pi}{3}\right) + \tilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\tilde{a}}\tilde{x}\right)\cos\left(\frac{2\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right) + \right)$$

611
$$\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{x}-\frac{\pi}{6}\right)\cos\left(\frac{2\pi}{\tilde{a}}\sqrt{3}\tilde{y}\right)\right) - \tilde{U}_{22}'\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{x}-\frac{2\pi}{3}\right),$$
(3.28)

612
$$-\frac{\partial \widetilde{U}}{\partial \widetilde{y}} = \widetilde{U}_{10}'\sqrt{3}\cos\left(\frac{2\pi}{3\widetilde{a}}\widetilde{x} + \frac{\pi}{3}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{U}_{11}'2\sqrt{3}\sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) -$$

613
$$\sqrt{3}\widetilde{U}_{20}'\sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\cos\left(\frac{4\pi}{3\widetilde{a}}\widetilde{x}+\frac{2\pi}{3}\right)+\widetilde{U}_{12}'\left(2\sqrt{3}\cos\left(\frac{2\pi}{\widetilde{a}}\widetilde{x}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)-$$

614
$$3\sqrt{3}\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{x}-\frac{\pi}{6}\right)\sin\left(\frac{2\pi}{\tilde{a}}\sqrt{3}\tilde{y}\right)\right)+2\sqrt{3}\tilde{U}_{22}'\sin\left(\frac{8\pi}{3\tilde{a}}\sqrt{3}\tilde{y}\right),$$
(3.29)

615 where the notations are introduced: 616

617
$$\tilde{U}_{10}' = \frac{8\pi}{3\tilde{a}}\tilde{V}_{1,(10)}, \quad \tilde{U}_{11}' = \frac{8\pi}{3\tilde{a}}\tilde{V}_{1,(11)}, \quad \tilde{U}_{20}' = \frac{16\pi}{3\tilde{a}}\tilde{V}_{1,(20)}, \quad \tilde{U}_{12}' = \frac{8\pi}{3\tilde{a}}\tilde{V}_{1,(12)}, \quad \tilde{U}_{22}' = \frac{16\pi}{3\tilde{a}}\tilde{V}_{1,(22)}.$$

618 (3.30)

620 Consider as the approximation the acting forces by $\tilde{t} = 0$, when $\tilde{\xi} = \tilde{x}$. After substitution 621 of (3.28) and (3.29) in (3.16), one obtains the expressions for the dimensionless forces 622 acting on the unit of mass of particles:

$$\begin{split} \widetilde{F}_{p\xi} &= -\frac{\partial \widetilde{\varphi}}{\partial \widetilde{\xi}} + \widetilde{U}_{10}' \sin\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{\pi}{3}\right) \cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{U}_{11}' \sin\left(\frac{4\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{\pi}{3}\right) - \\ 623 \qquad \widetilde{U}_{20}' \cos\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) \sin\left(\frac{4\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{2\pi}{3}\right) + \widetilde{U}_{12}' \left(6\sin\left(\frac{2\pi}{\widetilde{a}}\widetilde{\xi}\right)\cos\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right) + \\ &\cos\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{\pi}{6}\right)\cos\left(\frac{2\pi}{\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right) - \widetilde{U}_{22}' \sin\left(\frac{8\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{2\pi}{3}\right) + \widetilde{E}_{\xi}, \\ &\widetilde{F}_{py} = -\frac{\partial \widetilde{\varphi}}{\partial \widetilde{y}} + \widetilde{U}_{10}' \sqrt{3}\cos\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{\pi}{3}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{U}_{11}' 2\sqrt{3}\sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) - \\ &624 \qquad \sqrt{3}\widetilde{U}_{20}' \sin\left(\frac{4\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\cos\left(\frac{4\pi}{3\widetilde{a}}\widetilde{\xi} + \frac{2\pi}{3}\right) + \widetilde{U}_{12}' \left(2\sqrt{3}\cos\left(\frac{2\pi}{\widetilde{a}}\widetilde{\xi}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) - \\ &3\sqrt{3}\sin\left(\frac{2\pi}{3\widetilde{a}}\widetilde{\xi} - \frac{\pi}{6}\right)\sin\left(\frac{2\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right)\right) + 2\sqrt{3}\widetilde{U}_{22}' \sin\left(\frac{8\pi}{3\widetilde{a}}\sqrt{3}\widetilde{y}\right) + \widetilde{E}_{y}. \end{split}$$

625 Analogically

626

$$\widetilde{F}_{e\xi} = -\widetilde{F}_{p\xi}, \ \widetilde{F}_{ey} = -\widetilde{F}_{py}.$$
(3.33)

The forces (3.31)-(3.33) should be introduced in the system of the hydrodynamic equations (3.10)-(3.15).

629 Suppose that the external field intensity **E** is equal to zero. The effective 630 hydrodynamic velocity is directed along x axis. This fact can be used by averaging over \tilde{y} 631 of the obtained system of quantum hydrodynamic equations. The averaging will be realized 632 in the limit of one hexagonal crystal cell. Carry out the integration of the left and right hand

631 of the obtained 1, 632 in the limit of one hexagonal crystal cell. Carry out the integration of the 633 sides of the hydrodynamic equations calculating the integral $\frac{1}{\sqrt{3}\tilde{a}} \int_{\frac{\sqrt{3}}{2}\tilde{a}}^{\frac{\sqrt{3}}{2}\tilde{a}} d\tilde{y}$ (see figure 1) and

634 taking into account that $\frac{1}{\sqrt{3}\tilde{a}}\int_{-\frac{\sqrt{3}}{2}\tilde{a}}^{\frac{\sqrt{3}}{2}\tilde{a}}\frac{\partial\psi}{\partial\tilde{y}}d\tilde{y} = 0$ because of system symmetry for arbitrary

function Ψ , characterizing the state of the physical system. We suppose also that by averaging all physical values (characterizing the state of the physical system) do not depend on \tilde{y} .

638 As result we have the following system of equations:

639 Dimensionless Poisson equation for the self-consistent potential $\tilde{\varphi}$ of the electric field:

$$640 \qquad \frac{\partial^2 \tilde{\varphi}}{\partial \tilde{\xi}^2} = -4\pi R \left\{ \frac{m_e}{m_p} \left[\tilde{\rho}_p - \frac{m_e H}{m_p \tilde{u}^2} \frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_p \left(\tilde{u} - 1 \right) \right) \right] - \left[\tilde{\rho}_e - \frac{H}{\tilde{u}^2} \frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_e \left(\tilde{u} - 1 \right) \right) \right] \right\}.$$
(3.34)

641

642 Continuity equation for the positive particles:643

$$\frac{\partial}{\partial \xi} \left[\tilde{\rho}_{p} (1 - \tilde{u}) \right] + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi} \left[\tilde{\rho}_{p} (\tilde{u} - 1)^{2} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \left(-\frac{\partial \tilde{\varphi}}{\partial \xi} + \tilde{U}_{11}' \sin \left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) \right] \right\} = 0$$
(3.35)

645 Continuity equation for electrons:

646

647

644

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

$$(3.36)$$

648 Momentum equation for the movement along the *x* direction: 649

$$\frac{\partial}{\partial \tilde{\xi}} \left\{ \left(\tilde{\rho}_{p} + \tilde{\rho}_{e} \right) \tilde{u} \left(\tilde{u} - 1 \right) + \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{p}_{p} + \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{p}_{e} \right\} -$$

$$650 \qquad \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \left(-\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \tilde{U}_{11}' \sin \left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) -$$

$$\tilde{\rho}_{e} E \left(\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) +$$

$$\begin{aligned} \frac{m_e}{m_p} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} \left[\frac{\partial}{\partial \xi} \left(2 \frac{V_{0_p}^2}{u_0^2} \tilde{p}_p (1-\tilde{u}) - \tilde{\rho}_p \tilde{u} (1-\tilde{u})^2 \right) - \frac{m_e}{m_p} \tilde{\rho}_p (1-\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) \right] \right\} + \\ \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} \left[\frac{\partial}{\partial \xi} \left(2 \frac{V_{0_e}^2}{u_0^2} \tilde{p}_e (1-\tilde{u}) - \tilde{\rho}_e \tilde{u} (1-\tilde{u})^2 \right) - \tilde{\rho}_e \tilde{u} (1-\tilde{u})^2 \right) - \tilde{\rho}_e \tilde{u} (1-\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) \right] \right\} + \\ \frac{H}{\tilde{u}^2} 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) \left(\frac{\partial}{\partial \xi} (\tilde{\rho}_p (\tilde{u}-1)) \right) + \\ \frac{H}{\tilde{u}^2} 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) \left(\frac{\partial}{\partial \xi} (\tilde{\rho}_e (\tilde{u}-1)) \right) - \\ 653 \quad \frac{m_e}{m_p} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^2} \frac{V_{0_p}^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_{0_e}^2}{u_0^2} \frac{\partial}{\partial \xi} (\tilde{\rho}_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{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \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{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) \tilde{\rho}_e \tilde{u} \right] \right\} + \\ \left\{ \frac{m_e}{m_p} \right\} \left\{ \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{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \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{U}_{22}' \sin \left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3} \right) \right) \tilde{\rho}_e \tilde{u} \right] \right\} = 0 \end{aligned}$$

Energy equation for the positive particles: 656

 $\frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_p \tilde{u}^2 (\tilde{u} - 1) + 5 \frac{V_{0p}^2}{u_0^2} \tilde{p}_p \tilde{u} - 3 \frac{V_{0p}^2}{u_0^2} \tilde{p}_p \right] -$

 $2\frac{m_e}{m_p}\tilde{\rho}_p E\left(-\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}+\tilde{U}_{11}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)-\tilde{U}_{22}'\sin\left(\frac{8\pi}{3\tilde{a}}\tilde{\xi}-\frac{2\pi}{3}\right)\right)\tilde{u}+$

657

$$\begin{split} \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}(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} - \right. \\ 659 \quad 5 \frac{V_{0p}^{4}}{u_{0}^{6}} \frac{\tilde{\rho}_{p}}{\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{\rho}_{p} \right) \left(-\frac{\partial \tilde{\varphi}}{\partial \xi} + 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) \right] \right\} + 2 \frac{H}{\tilde{u}^{2}} E \left(\frac{m_{e}}{m_{p}} \right)^{2} \left[-\frac{\partial \tilde{\varphi}}{\partial \xi} (\tilde{\rho}_{p} \tilde{u}(1-\tilde{u})) + \frac{2}{\tilde{u}^{2}} \frac{\partial \tilde{\varphi}}{\partial \xi} \tilde{\rho}_{p} \right] \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 \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) \right] \right\} + 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] \right) - 2 \frac{H}{\tilde{u}^{2}} E^{2} \left(\frac{2\pi}{m_{p}} \right)^{3} \tilde{\rho}_{p} \left[\left(-\frac{\partial \tilde{\varphi}}{\partial \xi} + \tilde{U}_{11} \sin\left(\frac{2\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] \right)^{2} + \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 - \frac{\pi}{3}\right) - \tilde{U}_{22} \sin\left(\frac{8\pi}{3\tilde{a}} \xi - \frac{2\pi}{3}\right) \right)^{2} + \frac{1}{2} \left(\tilde{U}_{10} \sin\left(\frac{2\pi}{3\tilde{a}} \xi + \frac{\pi}{3}\right) - \frac{1}{2\tilde{u}} \tilde{U}_{12} \tilde{U}_{12} \sin\left(\frac{2\pi}{3\tilde{a}} \xi + \frac{\pi}{3}\right) - \frac{6\tilde{U}_{12} \sin\left(\frac{2\pi}{3\tilde{a}} \xi + \frac{\pi}{3}\right) + 2\tilde{U}_{12} \sin\left(\frac{2\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) \right)^{2} + 2\tilde{U}_{12} \cos\left(\frac{2\pi}{\tilde{a}} \xi + \frac{\pi}{3}\right) \cos\left(\frac{2\pi}{3\tilde{a}} \xi - \frac{\pi}{6}\right) + 6 \tilde{U}_{12} \right)^{2} + \frac{3}{2} \left(\tilde{U}_{11} - \tilde{U}_{12} \cos\left(\frac{4\pi}{3\tilde{a}} \xi + \frac{2\pi}{3}\right) \right)^{2} + 2\tilde{U}_{12} \left(\tilde{U}_{12} \sin\left(\frac{2\pi}{3\tilde{a}} \xi - \frac{\pi}{6}\right) + 6 \tilde{U}_{12} \left(\tilde{U}_{12} \cos\left(\frac{2\pi}{3\tilde{a}} \xi + \frac{\pi}{3}\right) + 2\tilde{U}$$

Energy equation for electrons:

$$\begin{array}{ll} & \frac{\partial}{\partial \xi} \left[\tilde{\rho}_{\epsilon} \tilde{u}^{2} (\tilde{u}-1) + 5 \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{\rho}_{\epsilon} \tilde{u} - 3 \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{\rho}_{\epsilon} \right] - \\ & 2 \tilde{\rho}_{\epsilon} \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}_{\epsilon} \tilde{u}^{2} (1 - \tilde{u})^{2} + 7 \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} \tilde{u} (1 - \tilde{u}) + 3 \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} (\tilde{u} - 1) - \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} \tilde{u}^{2} - \\ & \frac{\partial}{\partial \xi'} \left[\frac{\partial}{\partial \xi} \left(- \tilde{\rho}_{\epsilon} \tilde{u}^{2} (1 - \tilde{u})^{2} + 7 \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} \tilde{u} (1 - \tilde{u}) + 3 \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} (\tilde{u} - 1) - \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} \tilde{u}^{2} - \\ & \frac{\partial}{\partial \xi'} \left[\frac{\partial}{\partial \xi} \left(- \tilde{\rho}_{\epsilon} \tilde{u}^{2} (1 - \tilde{u}) \right) + 7 \frac{H}{\tilde{\mu}^{2}} \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \tilde{p}_{\epsilon} \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\} + \\ & E \left[-2 \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \xi'} \left(\tilde{\rho}_{\epsilon} \tilde{u} (1 - \tilde{u}) \right) + 2 \frac{H}{\tilde{u}^{2}} \frac{V_{u_{2}}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \xi'} \tilde{p}_{\epsilon} \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) - \\ & 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{2\pi}{3}\right) - \tilde{U}_{22}' \sin\left(\frac{8\pi}{3\tilde{a}} \tilde{\xi} - \frac{2\pi}{3}\right) \right]^{2} + \\ & \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}{3}\right) + \\ & \frac{1}{2} \left(\tilde{U}_{10}' \sin\left(\frac{2\pi}{\tilde{a}} \tilde{\xi} + \frac{2\pi}{3}\right) - \frac{4}{3\pi} \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{1}{2} \left(\tilde{U}_{10}' \cos\left(\frac{2\pi}{\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{1}{2} \left(\tilde{U}_{10}' \cos\left(\frac{2\pi}{\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{1}{2} \left(\tilde{U}_{10}' \cos\left(\frac{2\pi}{\tilde{a}} \tilde{\xi} + \frac{\pi}{3}\right) + 2 \tilde{U}_{12}' \cos\left(\frac{2\pi}{\tilde{a}} \tilde{\xi}\right$$

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$$670 \qquad \frac{72}{5\pi} \tilde{U}_{12}' \left(2\tilde{U}_{11}' - \tilde{U}_{02}' \cos\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi} + \frac{2\pi}{3}\right) \right) \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{6}\right) - \frac{288}{7\pi} \tilde{U}_{12}' \tilde{U}_{22}' \sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi} - \frac{\pi}{6}\right) \right] = 671 \qquad -\frac{\tilde{u}^2}{Hu_0^2} \left(V_{0e}^2 \tilde{p}_e - V_{0p}^2 \tilde{p}_p \right) \left(1 + \frac{m_p}{m_e} \right)$$
(3.39)

674

673 4. ESTIMATIONS OF THE NUMERICAL PARAMETERS

We need estimations for the numerical values of dimensionless parameters for solutions of the hydrodynamic equations (3.34) - (3.39). In its turn these parameters depend on choosing of the independent scales of physical values. Analyze the independent scales for the physical problem under consideration. It should be stressed that we choose just scales but not real physical values which may differ significantly from scale values. Real physical values will be obtained as a result of numerical self-consistent calculations.

Assume that the surface electron density in graphene is about $\tilde{n}_e \approx 10^{10} cm^{-2}$ (such value is typical for many experiments (see [35-37]), 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 (3.34)-(3.39) we need Cauchy conditions, obviously in the typical for graphene conditions the estimation $\tilde{\rho}_e \sim 1$ is valid which can be used as the condition by $\tilde{\xi} = 0$.

688 The process of the carbon atoms polarization leads to displacement of the atoms 689 from the regular chain and to the creation of the "effective" positive particles which 690 concentration $n_p \approx n_e$. Masses of these particles is about the mass of the carbon atom

691
$$m_p \approx 2 \cdot 10^{-23} c$$
. 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

692 choosed scale for the density ρ_0 we have $\tilde{\rho}_p \sim 2 \cdot 10^4$.

693 Going to the scales for thermal velocities for electrons and the positive particles we 694 have by T=300 K:

695
$$V_{0e} \sim \sqrt{\frac{k_B T}{m_e}} \approx 6.4 \cdot 10^6 \ cm/c$$
, take the scale $V_{0e} = 5 \cdot 10^6 \ cm/s$;

696
$$V_{0p} \sim \sqrt{\frac{k_B T}{m_p}} \approx 4.5 \cdot 10^4 \, c_M/c$$
, take the scale $V_{0p} = 5 \cdot 10^4 \, c_M/s$

697 The theoretical mobility in graphene reaches up to $10^6 cm^2/V \cdot s$ [38]. Let us use the scale

698
$$u_0 = 5 \cdot 10^6 \, cm \, s$$
. Then $N = \frac{V_{0e}^2}{u_0^2} = 1$, $P = \frac{V_{0p}^2}{u_0^2} = 10^{-4}$

699 Let us estimate the parameters *E* and *R*. For this estimation we need the scale
$$\varphi_0$$

Admit $\varphi_0 \approx \delta \frac{e}{a}$, where δ is a "shielding coefficient". Naturally to take $x_0 = a = 0.142$ nm

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(see figure 1) as the length scale, then $\tilde{a} = 1$. In the situation of a uncertainty in φ_0 choosing let us consider two limit cases:

703 1) δ~1.

704 Then
$$E = \frac{e\varphi_0}{m_e u_0^2} \sim 1000, \ R = \frac{e\rho_0 x_0^2}{m_e \varphi_0} \sim 3 \cdot 10^{-7}$$

706 Then
$$E = \frac{e\varphi_0}{m_e u_0^2} \sim 0.1$$
, $R = \frac{e\rho_0 x_0^2}{m_e \varphi_0} \sim 3.10^{-3}$

707 Consider the terms describing the lattice influence. We should estimate the 708 coefficients (3.30) using φ_0 as the scale for the potential *V*, $V = \varphi_0 \tilde{V}$. Three possible 709 cases under consideration:

710 1)
$$V \sim \varphi_0$$

711 We choose $U = \tilde{U}'_{10} \sim 10$, $F = \tilde{U}'_{11} \sim 10$, $J = \tilde{U}'_{20} \sim \pm 5$, $B = \tilde{U}'_{12} \sim \pm 2.5$, $G = \tilde{U}'_{22} \sim \pm 5$.

In this case the coefficients of "the second order" are less than the coefficients of "the first order."

714 2) $V \prec \varphi_0$ (The small influence of the lattice),

715 We choose
$$U = \tilde{U}'_{10} \sim 0.1$$
, $F = \tilde{U}'_{11} \sim 0.1$, $J = \tilde{U}'_{20} \sim 0.05$, $B = \tilde{U}'_{12} \sim 0.025$, $G = \tilde{U}'_{22} \sim 0.05$.

716 3)
$$V \succ \varphi_0$$
 (The great influence of the lattice),

717 We choose
$$U = \tilde{U}'_{10} \sim 1000$$
, $F = \tilde{U}'_{11} \sim 1000$, $J = \tilde{U}'_{20} \sim 500$, $B = \tilde{U}'_{12} \sim 250$, $G = \tilde{U}'_{22} \sim 500$.

Estimate parameter
$$H = \frac{N_R n}{m_e x_0 u_0}$$
 for two limit cases:

719 1)
$$N_R = 1$$
, then $H \sim 15$.

720 2) $N_R = 100$, then H~1500.

121 Initial conditions demand also the estimations for the quantum electron pressure and 122 the pressure for the positive species. For the electron pressure we have $p_e = \rho_0 V_{0e}^2 \tilde{p}_e$ and 123 using for the 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 $\tilde{p}_e \sim 1$. 124 Analogically for the positive particles $p_p = \rho_0 V_{0p}^2 \tilde{p}_p$, and using 125 $p_p = n_p k_B T \sim n_p m_p V_{op}^2 = \rho_p V_{0p}^2$, we have $p_p \sim 2 \cdot 10^4 \rho_0 V_{0p}^2$, $\tilde{p}_p \sim 2 \cdot 10^4$.

Tables 1, 2 contain the initial conditions and parameters which were not varied by
the numerical modeling.

729 730

718

Table 1. Initial conditions.

$ ilde{ ho}_{_{e}}(0)$	${ ilde{ ho}}_{_{p}}(0)$	$\widetilde{arphi}(0)$	$\tilde{p}_{e}(0)$	$\tilde{p}_{p}(0)$	$rac{\partial ilde{ ho}_{_e}}{\partial ilde{\xi}}(0)$	$rac{\partial \widetilde{ ho}_{_p}}{\partial \widetilde{\xi}}(0)$	$\frac{\partial \widetilde{\varphi}}{\partial \widetilde{\xi}}(0)$	$rac{\partial \widetilde{p}_{_{e}}}{\partial \widetilde{\xi}}(0)$	$rac{\partial {\widetilde p}_{_p}}{\partial {\widetilde \xi}}(0)$
1	$2 \cdot 10^4$	1	1	$2 \cdot 10^4$	0	0	0	0	0

731

Table 2. Constant parameters.

ã	L	Т	Ν	Ρ
1	1	$2 \cdot 10^{4}$	1	10^{-4}

734

Table 3 contains parameters (for the six different cases) which were varied by the numerical
 modeling.

737 738

Table 3. Varied parameters

Variant №	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
4	1000	$3 \cdot 10^{-7}$	15	10	10	5	2.5	5
5	0.1	0.003	1500	10	10	5	2.5	5
6	0.1	0.003	15	1000	1000	500	250	500

739

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.

745 5. RESULTS OF THE MATHEMATICAL MODELING WITHOUT THE EXTERNAL 746 ELECTRIC FIELD

747

The calculations are realized on the basement of equations (3.34)-(3.39) 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 (3.34) – (3.39)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 mathematical software Maple (beginning with the version 9) is applicable; the following Maple notations on figures are used: r- density $\tilde{\rho}_p$, s - density $\tilde{\rho}_e$, u- velocity \tilde{u} , p - pressure \tilde{p}_p , 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 $\frac{\partial \tilde{u}}{\partial \tilde{\xi}}(0) = 0$, independent variable *t*

760 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 ($\xi = \tilde{x} - \tilde{t}$) 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.

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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 (3.25) 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 (3.25) with $|g_1| \le 2$, $|g_2| \le 2$ (then coefficients *U*, *F*, *J*, *B* and *G*).





798 The self-consistent potential $\tilde{\varphi}$ is practically constant in the soliton boundaries, 799 (figures 4, 8). The small grows of the positive particles pressure exists in the *x* direction.

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800 This effect can be connected with the hydrodynamic movement along x and "the 801 reconstruction" of the polarized particles in the soliton front.

802 Comparing the figures 2-5 and 6-9 we conclude that the calculation results in the 803 first and the second approximation do not vary significantly. Seemingly significant difference 804 of figures 2 and 6 on the edges of the domain has not the physical sense because 805 corresponds to the regions where $u \neq const$. Then the restriction of two successive 806 approximations is justified. Along with it the question about the convergence of the series 807 lives open because the first and the second approximations include only the restricted 808 quantity of terms of the infinite series with the 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).





825 In the comparison with Variant 1 the calculations in Variant 3 are realized for the 826 case with opposite signs in front of the coefficients of second order. In this case the 827 distortion of the left side of soliton is observed because by $\xi < 0$ the velocity \tilde{u} is not 828 constant. Then this kind of potential for lattice is not favorable for creation of the super-829 conducting structures.

830 Variant 2 (Table 3) correspond to diminishing of the lattice potential in 100 times by 831 the same practically self-consistent potential, (see figures 16 - 23). 832



(solid line); p - the positive particles pressure

(the first approximation, Variant 2).



833

834

836 (the first approximation, Variant 2).





From comparison of figures 2 - 9 and 16 - 23 follow that numerical diminishing of the lattice potential (by the practically the same value of the self-consistent potential) does not influence on soliton size. But at the same time the solitons gain the more symmetrical forms. Therefore namely the self-consistent potential plays the basic role in the soliton formation.

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





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The comparison of figures 2 - 5 and 24 - 27 indicates that in the first approximation the very significant increasing of the *H* value in 100 times leads to increasing of the soliton size only in two times without significant changing of the soliton structure. The comparison of calculations (see figures 6 and 28) in the second approximation leads to conclusion that the region (where the velocity \tilde{u} is constant) has practically the same size.

Consider now the calculations responding to Variant 4 (Table 3). Increasing in 10^4 887 times of the scale φ_0 denotes increasing the self consistent potential and the lattice 888 potential introduced in the process of the mathematical modeling. This case leads to the 889 drastic diminishing of the soliton size. Figures 32 - 35 demonstrate that in the calculations of 890 the first approximation the soliton size is ~ $10^{-4}a = 1.42 \cdot 10^{-12} cm$ and exceeds the nuclei 891 size only in several times. The positive kernel of the soliton decreasing in the less degree 892 893 and occupies now the half of the soliton size. It is no surprise because the low boundary of 894 this kernel size is the character size of the nuclei. Application of the second approximation for the lattice potential function in the mathematical modeling leads to the significant soliton 895 deformation but the same soliton size (see figures 36-39). 896

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915 The drastic increasing of the periodic potential of the crystal lattice (in hundred 916 times, see figures 40 – 48) in comparison with the self-consistent potential also leads to 917 diminishing of the soliton size. For the case Variant 6, Table 3 this size consists only 918 $\sim 10^{-2} a$. But this increasing does not lead to the relative increasing of the soliton kernel 919 and to the mentioned above the soliton deformation in the second approximation (see

920 figures 45 – 48). Figure 41 demonstrates the extremely high accuracy of the soliton stability, 921 the velocity fluctuation inside the soliton is only $\sim 10^{-16} \tilde{u}$.



929 (the first approximation, Variant 6).





6. 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 (3.10) - (3.15) 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 (3.34) - (3.39)):

Poisson equation for the self-consistent electric field:

955
$$\frac{\partial^2 \widetilde{\varphi}}{\partial \widetilde{\xi}^2} = -4\pi R \left\{ \frac{m_e}{m_p} \left[\widetilde{\rho}_p - \frac{m_e H}{m_p \widetilde{u}^2} \frac{\partial}{\partial \widetilde{\xi}} (\widetilde{\rho}_p (\widetilde{u} - 1)) \right] - \left[\widetilde{\rho}_e - \frac{H}{\widetilde{u}^2} \frac{\partial}{\partial \widetilde{\xi}} (\widetilde{\rho}_e (\widetilde{u} - 1)) \right] \right\}.$$
(6.1)
956 Continuity equation for the positive particles:

$$\frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{p} \left(1 - \tilde{u} \right) \right] + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{p} \left(\tilde{u} - 1 \right)^{2} \right] \right\} + \frac{m_{e}}{m_{p}} \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left\lfloor \frac{V_{0p}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{p} - \frac{m_{e}}{m_{p}} \tilde{\rho}_{p} E \left(-\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} + \tilde{U}_{11}' \sin \left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) + \tilde{E}_{0} \right) \right] \right\} = 0$$
(6.2)

$$\sum_{p_p} \rho_p E\left[-\frac{1}{\partial \tilde{\xi}} + O_{11} \sin\left(\frac{1}{3\tilde{a}} - \frac{1}{3}\right) + E_0\right]$$

$$\frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{e} (1 - \tilde{u}) \right] + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{e} (\tilde{u} - 1)^{2} \right] \right\} + \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{V_{0e}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{e} - \tilde{\rho}_{e} E \left(\frac{\partial \tilde{\varphi}}{\partial \tilde{\xi}} - \tilde{U}_{11}' \sin \left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{E}_{0} \right) \right] \right\} = 0$$
(6.3)

Momentum equation for the *x* direction:

$$\begin{aligned} \frac{\partial}{\partial \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{\rho}_{p} + \frac{V_{0c}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \right\} - \\ 962 \quad \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{\rho}_{e} 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{m_{e}}{m_{p}} \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial \tilde{\xi}}{\partial \xi} \left(2 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p} \left(1 - \tilde{u} \right) - \tilde{\rho}_{p} \tilde{u} \left(1 - \tilde{u} \right)^{2} \right) - \\ \frac{m_{e}}{m_{p}} \tilde{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \xi} \left(2 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{p} \left(1 - \tilde{u} \right) - \tilde{\rho}_{p} \tilde{u} \left(1 - \tilde{u} \right)^{2} \right) - \\ \frac{\partial \tilde{\xi}}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \xi} \left(2 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \left(1 - \tilde{u} \right) - \tilde{\rho}_{p} \tilde{u} \left(1 - \tilde{u} \right)^{2} \right) - \\ \tilde{\rho}_{e} \left(1 - \tilde{u} \right) 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) \right] \right\} + \\ \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \xi} \left(2 \frac{V_{0p}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \left(1 - \tilde{u} \right) - \tilde{\rho}_{p} \tilde{u} \left(1 - \tilde{u} \right)^{2} \right) - \\ \tilde{\rho}_{e} \left(1 - \tilde{u} \right) 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) \right] \right\} + \\ \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \xi} \left(2 \frac{\tilde{\rho}}{\tilde{u}^{2}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right] - \frac{\partial}{\partial \xi} \left\{ \frac{H}{\tilde{u}^{2}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right) \right] \right\} + \\ \frac{H}{\tilde{u}^{2}} \left\{ \frac{\partial}{\partial \tilde{\xi}} \left\{ - \tilde{U}_{11}' \sin \left(\frac{4\pi}{3\tilde{a}} \tilde{\xi} - \frac{\pi}{3} \right) - \tilde{E}_{0} \right) \left(\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right) \right\} + \\ \frac{H}{\tilde{u}^{2}} \left\{ \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right\} \right\} - \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right\} \right\} + \\ \frac{H}{\tilde{u}^{2}} \left\{ \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right\} \right\} - \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right\} \right\} - \\ \frac{\partial}{\partial \tilde{\xi}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\partial \tilde{\xi}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right\} \right\} + \\ \frac{\partial}{\tilde{u}^{2}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\tilde{u}^{2}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{\partial}{\tilde{u}^{2}} \left(\tilde{\rho}_{p} \tilde{u} \right) \right\} \right\} \right\} - \\ \frac{\partial}{\tilde{u}^{2}} \left\{ \frac{H}{\tilde{u}^{2}} \left[\frac{$$

Energy equation for the positive particles:

$$\begin{array}{l} \begin{array}{l} \frac{\partial}{\partial \xi} \left[\tilde{\rho}_{p} \tilde{u}^{2} (\tilde{u}-1) + 5 \frac{V_{0_{p}}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u} - 3 \frac{V_{0_{p}}^{2}}{u_{0}^{2}} \tilde{p}_{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}{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_{0_{p}}^{2}}{u_{0}^{2}} \tilde{\rho}_{p} \tilde{u} (1 - \tilde{u}) + 3 \frac{V_{0_{p}}^{2}}{u_{0}^{2}} \tilde{p}_{p} (\tilde{u} - 1) - \frac{V_{0_{p}}^{2}}{u_{0}^{2}} \tilde{p}_{p} \tilde{u}^{2} - \\ 971 \quad 5 \frac{V_{0_{p}}^{4}}{u_{0}^{4}} \frac{\tilde{\rho}_{p}}{\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_{0_{p}}^{2}}{u_{0}^{2}} \tilde{p}_{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{E}_{0} \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})) + \\ 972 \quad \frac{V_{0_{p}}^{2}}{u_{0}^{2}} \frac{\partial}{\partial \tilde{\xi}} \tilde{p}_{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{E}_{0} \right) - \\ 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) \right] + \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] = \\ 974 \quad - \frac{\tilde{u}^{2}}{\tilde{u}^{2}} \left(\tilde{v}_{e}^{2} \tilde{\rho}_{p} - \tilde{\rho}_{e} V_{0e}^{2} \left(1 + \frac{m_{p}}{m_{e}} \right) \right) \right) + 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) = \\ 975 \quad \text{Energy equation for electrons:} \\ 976 \quad \frac{\partial}{\partial \tilde{\xi}} \left[\tilde{\rho}_{e} \tilde{u}^{2} \left(\tilde{u} - 1 \right) + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \tilde{u} - 3 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \tilde{u} (1 - \tilde{u}) + 3 \frac{V_{0e}^{2}}{\eta_{e}^{2}} \tilde{\rho}_{e} (\tilde{u} - 1) - \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \tilde{u}^{2} - \\ \frac{\partial}{\partial \tilde{\xi}}^{2} \left[\tilde{u}^{2} \left(\tilde{u}^{2} \left(\tilde{u} - 1 \right) + 5 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \tilde{u}^{2} - 7 \frac{V_{0e}^{2}}{u_{0}^{2}} \tilde{\rho}_{e} \tilde{u}^{2} - 1 \right) -$$

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

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

978

$$2E^{2}\frac{H}{\tilde{u}^{2}}\tilde{\rho}_{e}\left[\left(-\frac{\partial\tilde{\varphi}}{\partial\tilde{\xi}}+\tilde{U}_{11}'\sin\left(\frac{4\pi}{3\tilde{a}}\tilde{\xi}-\frac{\pi}{3}\right)+\tilde{E}_{0}\right)^{2}+\frac{1}{2}\left(\tilde{U}_{10}'\sin\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right)^{2}+\frac{3}{2}\left(\tilde{U}_{10}'\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right)^{2}+\frac{1}{2}\left(\tilde{U}_{10}'\tilde{\xi}+\frac{\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)^{2}+\frac{6}{2}\left(\tilde{U}_{10}'\tilde{U}_{11}'\right)\cos\left(\frac{2\pi}{3\tilde{a}}\tilde{\xi}+\frac{\pi}{3}\right)\right]=-\frac{\tilde{u}^{2}}{Hu_{0}^{2}}\left(V_{0e}^{2}\tilde{p}_{e}-V_{0p}^{2}\tilde{p}_{p}\right)\left(1+\frac{m_{p}}{m_{e}}\right)$$
(6.6)

Two classes of parameters were used by the mathematical modeling - parameters 980 and scales which were not changed during calculations and varied parameters indicated in 981 982 Table 4.

Parameters, scales and Cauchy conditions which are common for modeling with the 983 984 external field:

985
$$\frac{m_e}{m_p} = 5 \cdot 10^{-5}$$
, the scales $\rho_0 = 10^{-10} g/cm^3$, $u_0 = 5 \cdot 10^6 cm/s$, $V_{0e} = 5 \cdot 10^6 cm/s$,

986
$$V_{0p} = 5 \cdot 10^4 \text{ cm/s}$$
, $x_0 = a = 0.142 \text{ nm}$, $\varphi_0 = 10^{-4} \frac{e}{a} = 3.4 \cdot 10^{-6} \text{ CGSE}_{\varphi}$

Dimensionless parameters $R = 3 \cdot 10^{-3}$, E=0.1, H = 15 (by $N_R = 1$). Admit that for the lattice 987

988
$$U \sim V_{1,(10)} \sim V_{1,(11)} \sim \varphi_0$$
 and choose $U'_{10} = 10$, $U'_{11} = 10$.

Cauchy conditions $\tilde{\rho}_e(0) = 1$, $\tilde{\rho}_p(0) = 2 \cdot 10^4$, $\tilde{p}_e(0) = 1$, $\tilde{p}_p(0) = 2 \cdot 10^4$, $\tilde{\varphi}(0) = 1$, 989 **∽~** ລ~ (0) = 0.

990
$$\frac{\partial \rho_e}{\partial \tilde{\xi}}(0) = 0, \ \frac{\partial \rho_p}{\partial \tilde{\xi}}(0) = 0$$

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

991 992

Variant №	\widetilde{E}_{0}	$rac{\partial ilde{arphi}}{\partial ilde{\xi}}(0)$	$rac{\partial {\widetilde p}_{_p}}{\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

. . .

993

994 The external intensity of the electric field is written as
995
$$E_0 = \frac{\varphi_0}{x_0} \tilde{E}_0 = 10^{-4} \frac{e}{a^2} \tilde{E}_0 = 238CGSE_E \tilde{E}_0 = 7.14 \cdot 10^6 \frac{V}{m} \tilde{E}_0$$
. It means that even by

 $\widetilde{E}_0 = 1$ we are dealing with the rather strong fields. But namely strong external fields can 996 997 exert the influence on the soliton structures compared with the Coulomb forces in the lattice. For example in [39] the influence of the external electric field in graphene up to 998

999 $10^7 - 10^8 V/m$ is considered. The values \tilde{E}_0 are indicated in Table 4, variants 9.0 and 9.1 respond to the extremely strong external field.

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 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 correspond to $\tilde{E}_0 = 100$, figures 69 – 80 correspond to $\tilde{E}_0 = 10000$.

1007







1009 Figure 49. r – the positive particles density,

1010 (solid line); p – the positive particles pressure.

1011 (Variant 7.0).























1134 CDW expansion as well as the problem of the high temperature superconduction can be 1135 solved only on the basement of the nonlocal guantum hydrodynamics in particular on the 1136 basement of the Alexeev non-local quantum hydrodynamics. It is known that the 1137 Schrödinger - Madelung quantum physics leads to the destruction of the wave packets and can not be used for the solution of this kind of problems. The appearance of the soliton 1138 solutions in mathematics is the rare and remarkable effect. As we see the soliton's 1139 appearance in the generalized hydrodynamics created by Alexeev is an "ordinary" oft-1140 recurring fact. The realized here mathematical modeling CDW expansion support 1141 1142 established in [22, 24] mechanism of the relay ("estafette") motion of the soliton' system ("lattice ion - electron") which is realizing without creation of additional chemical bonds. 1143 Important to underline that the soliton mechanism of CDW expansion in graphene (and other 1144 1145 substances like NbSe₂) takes place in the extremely large diapason of physical parameters. But CDW existence belongs to effects convoving the high temperature 1146

superconductivity. It means that the high temperature superconductivity can be explained in 1147 the frame of the non-local soliton quantum hydrodynamics. 1148

Important to underline that the problem of existing and propagation of solitons in 1149 1150 graphene and in the perspective high superconducting materials belong to the class of 1151 significantly non-local non-linear problems which can be sold only in the frame of vast 1152 numerical modeling. 1153

REFERENCES 1154

1155

1156	[1] Alekseev, B.V. (1982). Matematicheskaya Kinetika Reagiruyushchikh Gazov.
1157	(Mathematical Theory of Reacting Gases) Moscow, Nauka.

1158 [2] Alexeev, B.V. (1994) The Generalized Boltzmann Equation, Generalized Hydrodynamic Equations and their Applications, Phil. Trans. Roy. Soc. Lond. Vol. 349, 417-443. 1159 1160 doi:10.1098/rsta.1994.0140

- [3] Alexeev, B.V. (1995). The Generalized Boltzmann Equation, Physica A, Vol. 216, 459 -1161 468. doi:10.1016/0378-4371(95)00044-8 1162
- 1163 [4] Alekseev, B.V. (2000). Physical Basements of the Generalized Boltzmann Kinetic Theory of Gases, Physics-Uspekhi, Vol. 43, No 6, 601 - 629. 1164 doi:10.1070/PU2000v043n06ABEH000694 1165
- [5] Alekseev, B.V. (2003). Physical Fundamentals of the Generalized Boltzmann Kinetic 1166 Theory of Ionized Gases, Physics-Uspekhi, Vol 46, No 2, 139 – 167. 1167 1168
 - doi:10.1070/PU2003v046n02ABEH001221
- 1169 [6] Alexeev, B.V. (2004) Generalized Boltzmann Physical Kinetics. Elsevier, Amsterdam, The Netherlands. 1170
- 1171 [7] Alexeev, B.V. (2008). Generalized Quantum Hydrodynamics and Principles of Non-Local 1172 Physics", J. Nanoelectron. Optoelectron. No. 3, 143 - 158. 1173 doi:10.1166/jno.2008.207
- 1174 [8] Alexeev, B.V. (2008). Application of Generalized Quantum Hydrodynamics in the Theory 1175 of Quantum Soliton Evolution", J. Nanoelectron. Optoelectron. No. 3, 316 - 328. 1176 doi:10.1166/jno.2008.311
- [9] Alexeev, B.V. (2012) Application of Generalized Non-Local Quantum Hydrodynamics to 1177 the Calculation of the Charge Inner Structures for Proton and Electron" Journal of 1178 1179 Modern Physics, 3, 1895-1906 doi:10.4236/jmp.2012.312239 Published Online 1180 December 2012 (http://www.SciRP.org/journal/jmp)
- [10] Alexeev, B.V. (2012) To the Theory of Galaxies Rotation and the Hubble Expansion in 1181 the Frame of Non-Local Physics" Journal of Modern Physics, 3, 1103-1122 1182 doi:10.4236/jmp.2012.329145 Published Online September 2012 1183
- 1184 (http://www.SciRP.org/journal/jmp)

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E-mail address: xyz@abc.com.

1185 [11] Boltzmann, L. (1872) Weitere Studien über das Wärmegleichgewicht unter 1186 Gasmolekulen, Sitz. Ber. Kaiserl. Akad. Wiss. 66 (2), 275. 1187 [12] Boltzmann, L. (1912) Vorlesungen über Gastheorie, Leipzig: Verlag von Johann Barth. 1188 [13] Chapman, S. and Cowling, T.G. (1952). The Mathematical Theory of Non-uniform 1189 Gases, Cambridge: At the University Press. 1190 [14] Hirschfelder, I.O., Curtiss, Ch. F. and, Bird, R.B. (1954). Molecular Theory of 1191 Gases and Liquids, John Wiley and sons, inc. New York. Chapman and Hall, lim., 1192 London. 1193 [15] Bell, J.S. (1964) On the Einstein Podolsky Rosen Paradox, Physics, v. 1, 195 - 200. 1194 [16] Madelung, E. (1927). Quantum Theory in Hydrodynamical Form", Zeit. f. Phys. 40, 1195 322 - 325. doi:10.1007/BF01400372 1196 [17] Landau, L.D. (1932). Zur Theorie der Energieübertragung. II 2, Physics of the Soviet 1197 Union, 46 - 51. 1198 [18] Zener, C. (1932). Non-adiabatic Crossing of Energy Levels. Proceedings of the Royal 1199 Society of London A 137 (6), 696-702. Bibcode 1932RSPSA.137..696Z. 1200 doi:10.1098/rspa.1932.0165. JSTOR 19320901 1201 [19] Gell-Mann, M. and Low, F. (1951). Bound States in Quantum Field Theory, Phys. 1202 Rev., 84, 350. doi:10.1103/PhysRev.84.350 1203 [20] Berry, M.V. (1984). Quantal Phase Factors Accompanying Adiabatic Changes. Proc. 1204 Royal Soc. London A, 392, 45. doi:10.1098/rspa.1984.0023 1205 [21] Simon, B. (1983) Holonomy, the Quantum Adiabatic Theorem and Berry's Phase, Phys. 1206 Rev. Letters, 51, 2167 - 2170. doi:10.1103/PhysRevLett.51.2167 1207 [22] Alexeev, B.V. (2012). To the Non-Local Theory of the High Temperature 1208 Superconductivity. ArXiv: 0804.3489 [physics.gen-ph] Submitted on 30 Jan 2012. 1209 [23] Алексеев, Б.В. (2008). Обобщенная квантовая гидродинамика //Вестник МИТХТ. 1210 T.3. №3. C.3-19 (Alexeev, B.V. Generalized Quantum Hydrodynamics. Vestnik 1211 MITHT, in Russian). [24] Алексеев, Б.В. (2012). К нелокальной теории высокотемпературной 1212 1213 сверхпроводимости. Вестник МИТХТ, Т. 7, №3, 3 – 21. (Alexeev, B.V. To the 1214 Non-Local Theory of the High Temperature Superconductivity. Vestnik MITHT, in 1215 Russian). 1216 [25]. Dürkop, T., Getty, S.A., Cobas, Enrique, and Fuhrer M.S., Nano Letters 4, 35 (2004)). 1217 [26] Kohsaka, Y., Hanaguri, T., Azuma M., Takano, M, Davis, J.C., Takagi, H. (2012). 1218 Visualization of the emergence of the pseudogap state and the evolution to 1219 superconductivity in a lightly hole-doped Mott insulator. Nature Physics. 8. 534 – 538. doi:10.1038/nphys2321 1220 1221 [27] Chang, J, Blackburn, E., Holmes, A.T., Christensen, N.B., Larsen, J., Mesot, J, Ruixing, 1222 Liang, Bonn, D.A., Hardy, W.N., Watenphul, A., v. Zimmermann, M., Forgan, E.M., 1223 Hayden, S.M. (2012). Direct observation of competition between superconductivity 1224 and charge density wave order in $YBa_2Cu_3O_y$. ArXiv:1206.4333[v2], 3 Jul 2012. 1225 Condensed Matter. Superconductivity. 1226 [28] Alexeev, B.V., Abakumov, A.I., Vinogradov, V.S., (1986). Mathematical Modeling of 1227 Elastic Interactions of Fast Electrons with Atoms and Molecules. Communications on 1228 the Applied Mathematics. Computer Centre of the USSR Academy of Sciences. 1229 Moscow. 1230 [29] Alexeev, B.V. (2011). Non-local Physics. Non-relativistic Theory, Lambert Academic 1231 Press (in Russian). 1232 [30] Лозовик, Ю.Е., Меркулова, С.П., Соколик, А.А. (2008). Коллективные электронные 1233 явления в графене//Успехи физических наук. Т.178. №7. 757-776. 1234 [31] Barlas, Y., Pereg-Barnea, T., Polini, M., Asgari, R., MacDonald, A.H. (2007) Chirality 1235 and Correlations in Graphene. Phys. Rev. Letters, 98, 236601. 1236 [32] Castro Neto, A.H., Guinea, F., Peres, N.M.R., Novoselov, K.S., Geim, A.K. (2009). The 1237 Electronic Properties of Graphene. Reviews of Modern Physics, 81,109-162.

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- 1238 [33] Vasko, F.T., Ryzhii, V. (2008) Photoconductivity of an intrinsic graphene.
- 1239 ArXiv,0801/3476v2 [cond-mat.mtrl-sci].
- [34] Alexeev, B.V. and Ovchinnikova, I.V. (2011). Non-local Physics. Relativistic Theory,
 Lambert Academic Press (in Russian).
- [35] Pisana, S., Lazzeri, M., Casiraghi, C., Novoselov, K.S., Geim, A.K., Ferrari, A.C., Mauri
 F. (2007). Breakdown of the adiabatic Born Oppenheimer approximation in
 graphene. Nature Materials. Vol.6, 198-201.
- [36] Завьялов, Д.В., Крючков, С.В., Тюлькина, Т.А. (2010). Численное моделирование
 эффекта выпрямления тока, индуцированного электромагнитной волной в
 графене. Физика и техника полупроводников 44, вып.7, 910-914 (Zavyalov, D.V.,
 Krychkov, S.V., Tyul'kina, T.A. Numerical simulation of the current rectification effect
 induced by an electromagnetic wave in graphene. Fisika and Tehnika
 Poluprovodnikov. in Russian)
- [37] Завьялов, Д.В., Крючков, С.В., Мещерякова, Н.Е. (2010). Влияние нелинейной
 электромагнитной волны на плотность тока в поверхностной сверхрешетке в
 сильном электрическом поле. Физика и техника полупроводников 39, вып.2, 214217. (Zavjalov, D.V., Kruchkov, S.V., Mestcheryakova, N.E. Influence of a nonlinear
 electromagnetic wave on the electric current density in a superficial superlattice in a
 strong electric field. Fisika i Tehnika Poluprovodnikov. in Russian)
- [38] Hwang, E.H., Adam, S., Sarma, S.D. (2007). Carrier transport in 2D graphene layers.
 ArXiv,0610157v2 [cond-mat.mes-hall].
- 1259 [39] Белоненко, М.Б., Лебедев, Н.Г., Пак, А.В., Янюшкина, Н.Н. (2011). Спонтанное
- 1260 поперечное поле в примесном графене. Журнал технической физики Т. 81. 1261 Вып.8.64-69. (Belonenko,M.B., Lebedev, N.G., Pak, A.V., Yanushkina, N.N.
- 1261 Вып.8.64-69. (Belonenko,M.B., Lebedev, N.G., Pak, A.V., Yanushkina, N.N.
 1262 Spontaneous transverse field in doped graphene. Journal of Technical Physics, in
 1263 Russian).