Modified hydrodynamic equations of quantum liquid, taking into account quantum shell effects

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Abstract. In this paper, the modified hydrodynamic equations of a quantum system consisting of a degenerate electron gas and a classical ion gas, which take into account quantum shell effects, are derived. Two approaches are considered. The first is based on the modification of hydrodynamic equations. The modified equations take into account the shell effects by introducing an additional external field into the equations of motion for the electronic component. The second approach is based on a simplified description of the DFT modeling of the electron distribution for a given ionic distribution. In deriving the self-consistent system of equations, the Green’s function method is used in the coordinate representation, previously successfully applied in analyzing quantum shell effects in a gas bubble of submicron size.

1. Introduction
Earlier in [1, 2], it was shown that in a mesoscopic system there are quantum shell effects (QSE), which are manifested in the existence of a non-heterogeneous electric field with a scale of non-uniformity of the order of the system size. The presence of this electric field leads to a nontrivial dynamic of compression of a gas bubble of submicron size, which differs from adiabatic compression.

In [1] to account for the QSE, it was proposed to introduce into the hydrodynamic equation of motion for the electronic component a term equal to \( eU_{\text{osc}} \frac{1}{n_e^{\text{free}}} \nabla p_e(n_e^{\text{free}}) \).

This approach allowed us to describe the equilibrium state of a gas bubble, in which the concentrations of electrons and ions are equal and coincide with the concentration of free noninteracting electrons in the potential well.

Also, this approach describes such a compression mode of a gas bubble, in which the compression time is significantly longer than the relaxation time of the ionic system to equilibrium density. Under such conditions, the compressible system is quasi-neutral, and the concentrations of electrons and ions coincide and have several points of extremum. This form of concentration of charged particles leads to the generation of shock waves and compression waves, which is fundamentally different from adiabatic compression.

2. Modification of equations
The most consistent way to model the hydrodynamic behavior of a system consisting of a degenerate electron gas and a classical ion gas while taking into account quantum shell effects is to use the
standard system of hydrodynamic equations for a gas of classical ions, DFT calculations for degenerate electrons, and the Poisson equation.

But this approach requires significant computational costs and is hardly applicable for macroscopic systems with a size of about a micron and a number of particles of the order of $10^{12}$. Therefore, in order to be able to analyze processes in such systems, it is necessary to develop more efficient methods of description.

In this work we consider two approaches to solve this problem.

The first approach is based on modification of hydrodynamic equations with electron quantum liquid specifically, the addition to the electron motion equation of an additional term characterizing the action of an external force.

\begin{align*}
\frac{\partial n_e}{\partial t} + \text{div}(n_e v_e) &= 0, \\
\frac{\partial v_e}{\partial t} + v_e \frac{\partial v_e}{\partial r} &= -\frac{1}{\rho_e} \frac{\partial p_e}{\partial r} + \frac{e}{m_e} \nabla \phi - \nabla U_e, \\
\frac{\partial n_i}{\partial t} + \text{div}(n_i v_i) &= 0, \\
\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial r} &= -\frac{1}{\rho_i} \frac{\partial p_i}{\partial r} - \frac{e}{m_i} \nabla \phi,
\end{align*}

where

\begin{equation}
p_e = \frac{(3\pi^2)^{2/3}}{5} \frac{\hbar^2}{m_e} (n_e)^{5/3}, \quad p_i = n_i k T_i,
\end{equation}

3. Hydrostatic equilibrium of compressed gas bubble. DFT calculations

To calculate distributions of electrons and ions in a spherically symmetrical bubble, we use DFT with spherical jellium background model and hydrostatic equation for ions [1, 2]. The method was described in detail in [1].

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

![Figure 1](image1.png)  
**Figure 1.** The density distributions of electrons (solid lines) and ions (dashed lines) for 10000 electrons at average density $10^{30}$ m$^{-3}$ (to the left) and $10^{31}$ m$^{-3}$ (to the right).
Quantum mechanical calculations can be applied for a relatively small number of particles \((N<10^5)\), so we need to use simpler method such as quantum electron fluid model [3] for larger number of particles. We will consider equation for quantum electron fluid without Bohm potential, but with oscillation potential \(U_{osc}\), which should reproduce density distribution obtained in DFT calculations

\[-\frac{1}{\rho_e} \nabla p_e + \frac{e}{m_e} \nabla \rho + \frac{e}{m_e} U_{osc} = 0.\]  
(5)

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

\[e \nabla U_{osc} \approx \frac{1}{n_e^{free}} \nabla p_e(n_e^{free}).\]  
(6)

4. Method using Green functions

The second approach is based on a simplified description of the DFT modeling of the electron distribution for a given ionic distribution. In this approach, we believe that the characteristic time for establishing the electronic distribution is substantially less than the characteristic times of the problem.

In substance, we only calculate the hydrodynamic motion of ions using the standard system of hydrodynamic equations.

\[\frac{\partial n_i}{\partial t} + div(n_i v_i) = 0,\]  
(7)

\[\frac{\partial v_i}{\partial t} + v_i \frac{\partial v_i}{\partial r} = -\frac{1}{\rho_i} \frac{\partial p_i}{\partial r} - \frac{e}{m_i} \nabla \phi,\]  
(8)

\[\frac{\partial \rho_i}{\partial t} + v_i \frac{\partial \rho_i}{\partial r} = -\frac{p_i}{\rho_i} \frac{\partial v_i}{\partial r} + \frac{2}{r} \frac{p_i}{\rho_i},\]  
(9)

\[p_i = n_i k T_i.\]  
(10)

The electric field arising due to quantum shell effects is calculated using the Poisson equation

\[\Delta \phi = -\frac{e}{\varepsilon_0} (n_i - n_e),\]  
(11)

where \(n_i\) is the ion number density, and \(n_e\) is the electron number density.

The electron density distribution is determined using Green function method in coordinate representation

\[n_e(r) = -\frac{2}{\pi} \int_{-\infty}^{\varepsilon_e} \text{Im} G(r, r, e) de.\]  
(12)

The Green function is determined from equation [4]

\[G(r'', r', e) = G_0 + \Delta G (r) + \int G_0 (r'', s, e) V(s) G_0 (r'', s, e) ds,\]  
(13)

\[G_0 (r'', r', e) = -\frac{m}{2 \pi \hbar^2 |r'' - r'|} \exp \left\{ \frac{i}{\hbar} |r'' - r'| p(r) \right\}, \quad r = \frac{r' + r''}{2},\]  
(14)

\[\Delta G (r'', r', e) = -\frac{1}{(2 \pi \hbar^2)^{3/2}} \sum_{\alpha} \left\{ p_{01} D^{1/2} \exp \left\{ \frac{i}{\hbar} S_{\alpha} (r'', r', e) + iv \frac{i\pi}{4} \right\} \right\},\]  
(15)

\[V(r) = e \phi(r).\]  
(16)

From (12) we have

\[\delta n_e^{free} = n_e^{free} - n_0 (r) = -\frac{2}{\pi} \int_{-\infty}^{\varepsilon_e} \text{Im} \Delta G(r, r, e) de.\]  
(17)
For quasiclassical approximation $\frac{i}{\hbar} p R_0 \gg 1$

\[ \int G_0 V G_0 d^3 r = V(r) \int G_0 G_0 d^3 r. \]  

(18)

Under assumption that $\Delta n/n_0 \ll 1$

\[ V(r) \int G_0 G_0 d^3 r \approx V(r) \alpha = e \varphi \alpha, \]  

(19)

where

\[ \alpha = \frac{3m_e n_0^{1/3}}{(3\pi^2)^{2/3} \hbar^2} \]  

(20)

\[ n_e \approx n_0 + \delta n_e^{\text{free}} - e \varphi \alpha \]  

(21)

From these equations we get modified Poisson equation

\[ \Delta \varphi = \frac{e}{\epsilon_0} \left( n_0 + \delta n_e^{\text{free}} - e \varphi \alpha - n_i \right) \]  

(22)

So, we obtain equation (22), which should be solved self-consistently with equations (7), (8) and (9). This is a closed system of equations that takes into account quantum shell effects.

5. Conclusion

In this paper, two approaches have been proposed for describing the hydrodynamic behavior of ions with allowance for quantum shell effects. The first approach is based on the modification of hydrodynamic equations. The modified equations take into account the shell effects by introducing an additional external field into the equations of motion for the electronic component.

The second approach is based on a simplified description of the DFT modeling of the electron distribution for a given ionic distribution.

In deriving the self-consistent system of equations, the Green's function method is used in the coordinate representation, previously successfully applied in analyzing quantum shell effects in a gas bubble of submicron size.

The considered approaches make it possible to significantly simplify the theoretical description of a quantum system as compared with the consistent approach, which describes the dynamics of electrons by DFT methods.

References

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