ABOUT FORMATION OF QUASIBOUND STATES AND ORDERED STRUCTURES IN DENSE PLASMA

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Abstract:

The possibility of formation of quasibound states and ordered structures in dense plasma is investigated. The effective potentials of dense plasma are used. On the basis of these models the condition of the ordered structures formation in the system is obtained. It is shown that in the dense classical plasma the quasibound states form whereas the ordered structures form in the dense semiclassical plasma.

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I. INTRODUCTION

It is well known\textsuperscript{1–4} that a classical Coulomb system form several ordered structures. As shown in Refs. 1 and 2, the strongly coupled one-component plasma will crystallize into a centered cubic form at the values of the coupling parameter $\Gamma \gg 1$. Here, $\Gamma = e^2/(ak_BT)$; $e$ is the electrical charge; $a = (3/4\pi n)^{1/3}$ is the average distance between particles (Wigner-Seitz radius); $n$ is the number density of particles; $k_B$ and $T$ are the Boltzmann constant and the temperature of plasma, respectively.

In previous papers\textsuperscript{3,4}, we studied the structural and thermodynamic properties of the two-component model plasma. The formation of the “near ordering” and anomalous increasing of the particle correlation radius as a consequence of microstructure changes in plasma have been demonstrated by Monte Carlo simulation method. The “hexatic”-like structures which characterized of liquid crystals were found in Refs. 5,6. In Refs. 7,8 the properties of the shell structures of finite one-component plasma clouds have been investigated. The study of ordered structures is especially important in connection with the rapid development of dusty plasma. The ordered structures that form in a strongly coupled plasma have been first analyzed theoretically in Ref. 9 and have come to be known as plasma crystals. The plasma crystals of dust particles were found also in a partially ionized plasma in a radio-frequency discharge\textsuperscript{10,11}, in the DC glow discharge\textsuperscript{12} and in the UV - induced dusty plasmas under microgravity\textsuperscript{13}.

It is now recognized that the plasma crystals are new material for future technologies. Therefore, the investigation of several ordered structures in Coulomb systems plays an important role.

II. INTERACTION MODELS

In this work we consider a fully ionized, dense (classical and semiclassical) hydrogen
plasma. The number density is considered in the range \( n = n_e = n_i \sim (10^{19} \div 2 \times 10^{25}) \text{ cm}^{-3} \), and the temperature domain is \( T \sim (5 \times 10^4 \div 10^6) \text{ K} \).

According to Ref. 14, we can separate two types of dense plasma. For example at \( \theta \gg 1 \) we have a classical dense plasma. Here \( \theta = k_B T / E_F \), \( k_B \) denotes the Boltzmann constant, \( T, E_F \) are a temperature and the Fermi energy, respectively. In this case, the quantum mechanical diffraction and symmetry effects are negligible except in short-range collisions. When \( \theta < 0,1 \), the electrons are in the state of full Fermi degeneracy. In the intermediate region between these cases \( (\theta \leq 1) \), the electrons are partially degenerate and we have a dense semiclassical plasma.

Due to the well known long range character of the Coulomb interaction between particles in plasma, the correlation effects play an important role for dense plasma. Consequently, for the dense plasma, the simultaneous interaction of a great number of particles should be taken into account. In Ref. 15, an integro-differential equation for the effective pair potential has been derived on the basis of Bogolyubov’s chain equation. This equation takes into account simultaneous correlations of \( N \) particles. In the case of three particle approximations the expression for the effective potential for dense plasma is\(^{15,16} \):

\[
\Psi(R) = \gamma \frac{e^{-R} 1 + \gamma f(R)/2}{1 + c(\gamma)}. \tag{1}
\]

Here \( f(R) = (e^{-\sqrt{\gamma} R} - 1)/(1 - e^{-2R})/5 \) and \( R = r/r_D \), where \( r_D \) is the Debye screening length. The potential is expressed in terms of the thermal energy, \( \Psi(R) = \Phi(R)/k_B T \), and \( \gamma = e^2/(r_D k_B T) \) is a nonideality plasma parameter. \( c(\gamma) \) is the correction coefficient for different values of \( \gamma \): \( c(\gamma) = -0.008617 + 0.455861 \gamma - 0.108389 \gamma^2 + 0.009377 \gamma^3 \).

For the semiclassical plasma, the effective potential of Kelbg-Deutsch-Yukhnovskii\(^ {17,18} \) is usually used:

\[
\Phi_{\alpha\beta}(r) = \frac{Z_\alpha Z_\beta e^2}{r} \left[ 1 - \exp(-r/\lambda_{\alpha\beta}) \right] + \tag{2}
\]
\[ \delta_{\alpha\beta}\delta_{\epsilon\alpha}k_B T \ln(2) \exp \left( -\frac{r^2}{\pi \ln(2) \lambda_{ee}^2} \right), \]

where \( \lambda_{\alpha\beta} = \hbar/(2\pi \mu_{\alpha\beta} k_B T)^{1/2} \) is the thermal de Broglie wavelength; \( \mu_{\alpha\beta} \) is the reduced mass of electrons and ions. Notice that the effective potential (2) does not account for screening effects in plasma and behaves like the Coulomb potential for \( r \to \infty \). Therefore, in Ref. 19, the effective semiclassical potential was obtained by applying the spline approximation to potential (2) and the numerical solution of following Equation 19:

\[ \Delta \Psi - 3\Gamma \Psi = \pm 3\Gamma \Psi^2, \]  

with the boundary conditions

\[ \Psi |_{R \to 0} = \Gamma / R; \quad \Psi |_{R \to \infty} = 0 \]  

at the intersection point.

The effective potential \( \Psi(R) \) is expressed in units of \( k_B T \) and \( R = r/a \); \( \Delta \) is the Laplace operator. In Equation (3) the minus and plus signs correspond to the interaction of particles with equal and opposite charges, respectively. The spline approximation was performed at the intersection point of Eq.(2) and the numerical solution of (3) – (4). This potential contains quantum diffraction and symmetry effects at short distances as well as screening effects for large distances (see Fig.1).

### III. ORDERED STRUCTURES IN DENSE PLASMA

Following 20, let us introduce a potential function for the mathematical description of the system state. This function takes into account the collective interaction between the components of statistical system:

\[ U(\vec{r}, \vec{v}, t) = \int \Phi(\vec{r}, \vec{v}, \vec{r}', \vec{v}'t) f(\vec{r}', \vec{v}'t) d\vec{r}' d\vec{v}'. \]  

Here \( \Phi(\vec{r}, \vec{v}, \vec{r}', \vec{v}'t) \) is the potential describing the interaction of particles in the system;
\( \vec{a}, \vec{v} \) are a coordinate and a velocity of particles, respectively.

If many-particles effects are considered (e.g. three particle effects), the expression for \( U(\vec{r}, \vec{v}, t) \) becomes non-linear:

\[
U(\vec{r}, t) = \int \Phi_{12}(|\vec{r} - \vec{r}'|) f(\vec{r}', \vec{v}, t) d\vec{r}' d\vec{v} + \int \int \Phi_{123}(|\vec{r} - \vec{r}'|, |\vec{r} - \vec{r}''|, |\vec{r}' - \vec{r}''|) f(\vec{r}', \vec{v}', t) f(\vec{r}'', \vec{v}'', t) d\vec{r}' d\vec{v}' d\vec{r}'' d\vec{v}''.
\]

In the case of pair central interaction between particles we can written as

\[
\Phi(\vec{r}, \vec{v}, \vec{r}', \vec{v}') = \Phi(|\vec{r} - \vec{r}'|).
\]

Taking into consideration Eq.(7), the expression for potential function is obtained:

\[
U(\vec{r}, t) = \int \Phi(|\vec{r} - \vec{r}'|) f(\vec{r}', \vec{v}, t) d\vec{r}' d\vec{v}.
\]

Considering the effective potentials and the field of collective interactions, we can obtain the following set of equations for the potential function \( U \) and plasma particles density function \( \rho \):

\[
U(\vec{r}) = C \int \Phi_{eff}(|\vec{r} - \vec{r}'|) e^{-U(\vec{r}')/\theta} d\vec{r}'
\]

\[
\rho(\vec{r}) = C \exp \left[ -\frac{1}{\theta} U(\vec{r}) \right],
\]

where \( \theta = 1/k_B T; \) \( C \) is the constant.

We consider the occurrence problem of space-periodical solution for Eq.(3). In this case, the expression for \( U(\vec{r}) \) can be written in the following form:

\[
\varphi(\vec{r}) = \lambda \int \Phi_{eff}(|\vec{r} - \vec{r}'|) e^{\varphi(\vec{r}')} d\vec{r}'
\]

where \( \varphi = -U/\theta; \lambda = -C/\theta. \) Let us that at \( \lambda = \lambda_0 \) and \( \varphi = \varphi_0 \) we have a violation of space-uniform solution. Let \( \lambda = \lambda_0 + \varepsilon, \varphi = \varphi_0 + u(\vec{r}) \) and the equation for \( u(\vec{r}) \) is written as:

\[
\varphi_0 + u(\vec{r}) = (\lambda_0 + \varepsilon) \int \Phi_{eff}(|\vec{r} - \vec{r}'|) e^{\varphi_0 + u(\vec{r}')} d\vec{r}',
\]
After expanding the element of integration as a power series in \( u(\vec{r}) \), we have the following expression:

\[
L[u(\vec{r})] = u(\vec{r}) - \lambda_0^* \int \Phi_{eff}(|\vec{r} - \vec{r}'|)u(\vec{r}')d\vec{r}',
\]  

where \( \lambda_0^* = \lambda_0 e^{\rho_0}; \sigma(0) = 4\pi \int_0^\infty \Phi(s)s^2 ds. \)

We consider the following linear equation

\[
u(\vec{r}) = \lambda_0 e^{\rho_0} \int \Phi_{eff}(|\vec{r} - \vec{r}'|)u(\vec{r}')d\vec{r}'.
\]  

According to the occurrence problem of periodical structures from homogeneous medium, the solution for \( u(\vec{r}) \) is sought as \( u(\vec{r}) = Ae^{ik\vec{r}} \). After inserting this solution into the Eq. (13) and integration, we have the following expression

\[
e^{ik\vec{r}} = \lambda_0 e^{\rho_0} \cdot e^{ik\vec{r}} \cdot 4\pi \int_0^\infty \Phi_{eff}(s) \frac{\sin(ks)}{ks}s^2 ds.
\]  

Consequently, in order that ordered structures in the system can form, it is necessary that the periodical solution of the following equation of nonlocal statistical mechanics to exist:

\[
\frac{\theta}{\rho} = -4\pi \int_0^\infty \Phi_{eff}(s) \cdot \frac{\sin(ks)}{ks}s^2 ds \equiv \sigma(k).
\]

In the present work, the behavior of the function \( \sigma(k) \) is investigated for the above mentioned models of dense plasma; here \( k \) is a wave number.

The model of dense classical plasma is characterized by the fact that for the low limit of integral (15) we must take a certain non-zero value of distance \( R_0 = r/r_D \). In this case, \( R_0 \) is minimal distance between particles. In Figure 2, the results of numerical analysis of expression (13) on the basis of effective potential (1) are shown. Notice that, with increasing of \( \gamma \), on the dependencies of \( \sigma(k) \) some non-monotonic behavior are observed. In this case, the increase of \( \gamma \) is caused by the density increase (the decreasing of \( r_D \)). It is well known that for a dense plasma the number of particles in Debye sphere \( N_D < 1 \). It is obtained also that functions \( \sigma(k) \) form local minimums when \( R_0 \sim 1 \) (\( r \approx r_D \)). These facts can be interpreted as the formation of quasibound states in dense classical plasma. The term ”quasibound” states\(^{21,22} \) denotes that the energy \( \varepsilon \) of electron-proton pairs is
\(-e^2/a < \varepsilon \leq 0\). Because the size of "quasibound" states is greater than \(a\), it is considered that the electron moves over a part of elliptical orbit in the field of the nearest proton, thereupon the electron passes into the field of another proton, and so on.

For the model of dense semiclassical plasma, the problem of introduction of minimal distance is absent because the pseudopotential (full line in Fig.1) is limited for \(r = 0\) and it is strongly screened when \(r \to \infty\). The results of numerical analysis of Eq. (15) are represented in Figures 3,4 and 5 for different values of the density parameter \(r_s = a/a_B\) and the coupling parameter \(\Gamma = Z_aZ_\beta e^2/(ak_BT)\). Here, \(a\) is the average distance between particles and \(a_B\) is the Bohr radius. It is shown that no oscillations on dependencies of \(\sigma_{ee}(k)\) for electron-electron component are observed. It is probably connected with the fact that electrons do not form complexes (structures) between themselves because of their little masses. The functions \(\sigma_{ep}\) and \(\sigma_{pp}\) have pronounced oscillations that can be considered as formation of ordered structures.

In Refs. 2,23 it has been demonstrated that in the intermediate region \((1 \leq \Gamma \leq 150)\) the plasma can be considered as a ordered structures of ions. According to this model, ions form a cubic-like space structures due to the strong interactions between particles. Since we have a chaotic motion in the system, these structures are realized "on the average". Therefore, the energy of this structure is greater then Madelung’s energy of simple centered cubic lattice. These configurations are called as "ordered structures".

Consequently in dense semiclassical hydrogen plasma, the “picture” of particles distribution can be as follows. Protons are distributed with a certain order and they are surrounded by electron clouds. The “proton-electron” system can be considered as a quasi-particle.

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Figure captions

Figure 1: Effective electron-proton potential for dense semiclassical hydrogen plasma at $r_s = 1$ and $\Gamma = 2$ (solid line). Triangles denote the numerical solution of Eq. (3) for a dense, classical plasma\textsuperscript{15} which accounts for higher-order screening effects. The dashed line denotes potential\textsuperscript{17,18} which shows quantum corrections at short distances. The dot-dashed line: DH potential.

Figure 2: Reduced $\sigma^*_\sigma = \sigma/(r_D^3 k_B T)$ functions for dense classical plasma at $R_0 = 2$.

Figure 3: Reduced $\sigma^*_{ee} = \sigma_{ee}/(a^3 k_B T)$ functions between electrons of dense semiclassical hydrogen plasma at $r_s = 5$.

Figure 4: Reduced $\sigma^*_{ep} = \sigma_{ep}/(a^3 k_B T)$ electron-proton functions of dense semiclassical hydrogen plasma at $r_s = 2$.

Figure 5: Reduced $\sigma^*_{pp} = \sigma_{pp}/(a^3 k_B T)$ functions between protons of dense semiclassical hydrogen plasma at $r_s = 1$. 
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Figure 3: Reduced $\sigma_{ee}^* = \sigma_{ee}/(a^3k_BT)$ functions between electrons of dense semiclassical hydrogen plasma at $r_s = 5$. 

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Figure 4: Reduced $\sigma_{ep}^* = \sigma_{ep}/(a^3 k_B T)$ electron-proton functions of dense semiclassical hydrogen plasma at $r_s = 2$. 
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Figure 5: Reduced $\sigma_{pp}^* = \sigma_{pp}/(a^3k_BT)$ functions between protons of dense semiclassical hydrogen plasma at $r_s = 1$. 