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Thermodynamics of dense high-temperature plasmas: Semiclassical approach

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Abstract. The pseudopotential model of particle interaction of a semiclassical fully ionized plasma, taking into account both quantum effects at short distances and screening field effects at large distances is developed. Radial distribution functions are investigated and it is shown that a short-range order formation can occur in the system under discussion. Correlation energy of dense high-temperature plasma, existing in astrophysical objects is studied and comparison with other methods is performed.

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1 Introduction

At the present time the importance of study of various properties of high-pressure plasmas has considerably increased. First of all it is a result of common interest in investigations of astrophysical plasmas such as the interiors of the main sequence stars (for which the Sun is a typical representative) and also neutron stars and white dwarfs which are the products of the final stages of stellar evolution. The concentration of charged particles in such formations can reach values of about $10^{24} \div 10^{28}$ cm^{-3} at temperature of about $10^5 \div 10^7$ K. It is quite natural that the properties of matter existing under such extreme conditions differ radically from the properties of a classical plasma. Quantum-mechanical effects of diffraction and symmetry on a level with plasma polarization effects play significant part in determining plasma characteristics.

In accordance with the aforesaid the investigations which allow to obtain reliable information about the properties of moderately coupled high-temperature plasma acquire great importance. Recently noticeable experimental progress has been made in this field [1–6]. All these laboratory experiments are based on the use of shock-waves generated both by explosive devices [1] and laser beams [2–6]. It should be mentioned here that thermodynamic [1–5] and transport [6] characteristics of samples compressed up to pressures of the order of 40 Mbar have been accurately measured in these tests. At the same time computer simulation methods [7] and also various theoretical approaches are widely used to determine high-pressure plasma properties. Among the most widespread ones are the Bogolyubov's method [8,9], the linear density-response formalism [10,11], the method of Green's functions [12], hypernetted-chain approximation [13], the Feynman-Kac path integral representation [14] and others. There also exist a tendency to use mixed approximation schemes. For instance, Chabrier and Potekhin [15] have applied the linear-response theory with local field corrections and the N-body hypernetted chain equations to determine thermodynamic quantities in a wide range of plasma parameters.

In this paper we restrict ourselves to consideration of results concerning fully ionized homogeneous plasma in which the influence of magnetic field can be omitted.

In the second section of this paper dimensionless values relevant to the description of characteristic parameters of dense high-temperature plasmas are introduced. In the third section the pseudopotential model of the particle interaction of semiclassical plasmas, taking into account both quantum-mechanical effects and screening field effects is developed. In section four the radial distribution functions are explored on the basis of the proposed model. Section five is devoted to the study of the internal energy of dense high-temperature plasma. Summarizing conclusions are formulated in the last section.

2 Plasma parameters

We consider the two-component high-temperature fully ionized plasma consisting of ions (electric charge Ze, mass m_i and number density n_i) and electrons (electric charge $-e$, mass m_e and number density $n_\mathrm{e} = Zn_\mathrm{i}$). Ionic subsystem of such plasma can be characterized by the average interparticle distance

$$a = \left(\frac{3}{4\pi n_\mathrm{i}}\right)^{1/3}, \qquad (1)$$

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and by the dimensionless Coulomb coupling parameter

$$\Gamma = \frac{(Ze)^2}{a k_{\mathrm{B}} T}, \tag{2}$$

where T is plasma temperature and k_{B} denotes the Boltzmann constant.

Here Γ is the ratio between average Coulomb interaction energy and thermal kinetic energy of ions. A weakly coupled plasma corresponds to the case $\Gamma < 1$ where the Coulomb interactions can be treated perturbation-theoretically and strongly coupled one refers to the case $\Gamma > 1$.

Electron subsystem can be described by the dimensionless density parameter

$$r_{\mathrm{s}} = \left(\frac{3}{4\pi n_{\mathrm{e}}}\right)^{1/3} \frac{m_{\mathrm{e}} e^2}{\hbar^2}, \tag{3}$$

and by the degeneracy parameter

$$\theta = \frac{k_{\mathrm{B}} T}{E_{\mathrm{F}}} = 2\left(\frac{4}{9\pi}\right)^{2/3} Z^{5/3} \frac{r_{\mathrm{s}}}{\Gamma}, \tag{4}$$

where E_{F} is the Fermi energy of electrons and $\hbar$ denotes the Plank constant. When $\theta \ll 1$ electrons are in the state of complete Fermi degeneracy and when $\theta \gg 1$ electrons subsystem can be treated within the classical physics approach. For the intermediate degeneracy $\theta \sim 1$ quantum-mechanical effects can be taken into consideration by introducing effective potentials (semiclassical approach).

The density parameter r_{s} represents the ratio between the mean inter-electron spacing and the Bohr radius. Thus, if $r_{\mathrm{s}} \leq 1$ then bound state effects must be properly included.

In this paper a dense high-temperature hydrogen plasma ($Z = 1$) is considered. It can be found in the interiors of the main sequence stars. Such plasma has the pressure of approximately 10^5 Mbar and the temperature of about 10^7 K. In these conditions the coupling, density and degeneracy parameters have magnitudes close to 1 (for the Sun $r_{\mathrm{s}} \sim 0.4$ and $\Gamma \sim 0.1$). Consequently not only polarization but also quantum-mechanical effects are essential for such plasma.

3 Pseudopotential model

It is well-known that there exist two principle difficulties arising in determination of both thermodynamic and transport properties of dense high-temperature plasmas. The first one is conditioned by long-range character of bare Coulomb interaction potential of charged particles. As a result, all theoretical approaches created for neutral gases can not be directly applied for the description of such plasma properties. As a rule, the above-mentioned difficulty is avoided by taking into consideration collective effects connected with great number of interacting particles (screening effects). On the other hand when plasma density increases the ratio between the average interparticle distance and the thermal de Broglie wavelength decreases and, therefore, the problem of inclusion of quantum-mechanical effects appears. In accordance with the aforesaid it is of great interest to construct the pseudopotential model of the particle interaction of dense high-temperature plasmas, taking into account both quantum-mechanical effects at short distances and the screening field effects at large distances.

To determine thermodynamic and transport properties of semiclassical fully ionized plasma effective potentials, simulating quantum effects of diffraction and symmetry are widely used. In particular, Deutsch and co-workers [16,17] have obtained the following form of effective interaction potential of charged particles in plasma medium:

$$\varphi_{\mathrm{ab}}(r) = \frac{e_{\mathrm{a}} e_{\mathrm{b}}}{r}\left[1 - \exp\left(-\frac{r}{\lambda_{\mathrm{ab}}}\right)\right] + \delta_{\mathrm{ae}}\delta_{\mathrm{be}} k_{\mathrm{B}} T \ln 2 \exp\left(-\frac{r^2}{\lambda_{\mathrm{ee}}^2 \pi \ln 2}\right), \tag{5}$$

where $e_{\mathrm{a}}, e_{\mathrm{b}}$ are the electric charges of interacting particles, $\lambda_{\mathrm{ab}} = \hbar/(2\pi\mu_{\mathrm{ab}} k_{\mathrm{B}} T)^{1/2}$ is the thermal de Broglie wavelength, $\mu_{\mathrm{ab}} = m_{\mathrm{a}} m_{\mathrm{b}}/(m_{\mathrm{a}} + m_{\mathrm{b}})$ is the reduced mass of a–b pair, δ_{ab} is the Kronecker delta.

The pseudopotential (5) does not take into account collective events in plasma. That is why Baimbetov *et al.* [18] proposed to use the effective potential (5) at short distances and the screened potential, treating three-particle correlations (see [8,9]) at large ones. The transition from one potential curve to the other was realized at the intersection point by the spline-approximation method.

In this regard, it is of great interest to obtain the analytical expression for the pseudopotential $\Phi_{\mathrm{ab}}(r)$, taking into account both quantum-mechanical effects of diffraction and symmetry and also screening field effects. In this paper we apply the classical approach based on the chain of Bogolyubov equations for the equilibrium distribution functions where the potential (5) is taken as a micropotential. Following [19] in the framework of the pair correlation approximation it is not difficult to deduce the following system of integral-differential equations for the pseudopotential $\Phi_{\mathrm{ab}}(r)$

$$\triangle_i \Phi_{\mathrm{ab}}({}^{\mathrm{a}}\mathbf{r}_i, {}^{\mathrm{b}}\mathbf{r}_j) = \triangle_i \varphi_{\mathrm{ab}}({}^{\mathrm{a}}\mathbf{r}_i, {}^{\mathrm{b}}\mathbf{r}_j) - \sum_{c=\mathrm{e,i}} \frac{n_c}{k_{\mathrm{B}} T} \int \mathrm{d}^c\mathbf{r}_{\mathrm{m}} \triangle_i \varphi_{\mathrm{ac}}({}^{\mathrm{a}}\mathbf{r}_i, {}^{c}\mathbf{r}_{\mathrm{m}}) \Phi_{c\mathrm{b}}({}^{c}\mathbf{r}_{\mathrm{m}}, {}^{\mathrm{b}}\mathbf{r}_j). \tag{6}$$

Here $\triangle_i$ denotes the Laplace operator acting on the coordinates of the ith particle.

In Fourier space this system of integral-differential equations turns into a system of linear algebraic equations. Solving this system for two-component plasma one can derive the following expressions for the Fourier transform $\tilde{\Phi}_{\rm ab}(k)$ of the pseudopotential $\Phi_{\rm ab}(r)$:

$$\tilde{\Phi}_{\rm ee}(k) = \frac{4\pi e^2}{\Delta}\left\{\frac{1}{k^2(1+k^2\lambda_{\rm ee}^2)} + \frac{1}{k^4 r_{\rm Di}^2}\left[\frac{1}{(1+k^2\lambda_{\rm ee}^2)(1+k^2\lambda_{\rm ii}^2)} - \frac{1}{(1+k^2\lambda_{\rm ei}^2)^2}\right] + A\left(1+\frac{1}{k^2 r_{\rm Di}^2(1+k^2\lambda_{\rm ii}^2)}\right)\exp\left(-\frac{k^2}{4b}\right)\right\}, \quad (7)$$

$$\tilde{\Phi}_{\rm ii}(k) = \frac{4\pi Z^2 e^2}{\Delta}\left\{\frac{1}{k^2(1+k^2\lambda_{\rm ii}^2)} + \frac{1}{k^4 r_{\rm De}^2}\left[\frac{1}{(1+k^2\lambda_{\rm ee}^2)(1+k^2\lambda_{\rm ii}^2)} - \frac{1}{(1+k^2\lambda_{\rm ei}^2)^2}\right] + \frac{A}{k^2 r_{\rm Di}^2(1+k^2\lambda_{\rm ii}^2)}\exp\left(-\frac{k^2}{4b}\right)\right\}, \quad (8)$$

$$\tilde{\Phi}_{\rm ei}(k) = -\frac{4\pi Z e^2}{\Delta}\frac{1}{k^2(1+k^2\lambda_{\rm ei}^2)}, \quad (9)$$

where $b = (\lambda_{\rm ee}^2 \pi \ln 2)^{-1}$, $A = k_{\rm B}T \ln 2\sqrt{\pi}b^{-3/2}/(4e^2)$, $r_{\rm De}$, $r_{\rm Di}$ are the Debye radius of electrons and ions respectively, and Δ is

$$\Delta = 1 + \frac{1}{k^2 r_{\rm De}^2(1+k^2\lambda_{\rm ee}^2)} + \frac{1}{k^2 r_{\rm Di}^2(1+k^2\lambda_{\rm ii}^2)} + \frac{1}{k^2 r_{\rm De}^2 k^2 r_{\rm Di}^2}\left[\frac{1}{(1+k^2\lambda_{\rm ee}^2)(1+k^2\lambda_{\rm ii}^2)} - \frac{1}{(1+k^2\lambda_{\rm ei}^2)^2}\right] + \frac{A}{r_{\rm De}^2}\left(1+\frac{1}{k^2 r_{\rm Di}^2(1+k^2\lambda_{\rm ii}^2)}\right)\exp\left(-\frac{k^2}{4b}\right). \quad (10)$$

Analogous expressions can be reached with the linear density-response formalism [10].

The pseudopotential $\Phi_{\rm ab}(r)$ can be restored from (7–10) by Fourier transformation

$$\Phi_{\rm ab}(r) = \frac{1}{(2\pi)^3}\int d\mathbf{k}\tilde{\Phi}_{\rm ab}(k)\exp(i\mathbf{k}\cdot\mathbf{r}). \quad (11)$$

Let us consider the limiting cases of the expressions (7–11).

A. $r_{\rm De}, r_{\rm Di} \to \infty$, then

$$\Phi_{\rm ab}(r) = \varphi_{\rm ab}(r). \quad (12)$$

In the absence of screening effects, the pseudopotential $\Phi_{\rm ab}(r)$ coincides with the potential (5).

B. $\lambda_{\rm ii}, \lambda_{\rm ei}, \lambda_{\rm ee} \to 0$, then

$$\Phi_{\rm ab}(r) = \frac{e_{\rm a}e_{\rm b}}{r}\exp\left(-\frac{r}{r_{\rm D}}\right), \quad (13)$$

where

$$\frac{1}{r_{\rm D}^2} = \sum_{c={\rm e,i}}\frac{4\pi n_c e_c^2}{k_{\rm B}T}\,. \quad (14)$$

In the absence of quantum-mechanical effects, the pseudopotential $\Phi_{\rm ab}(r)$ coincides with the Debye-Hückel one.

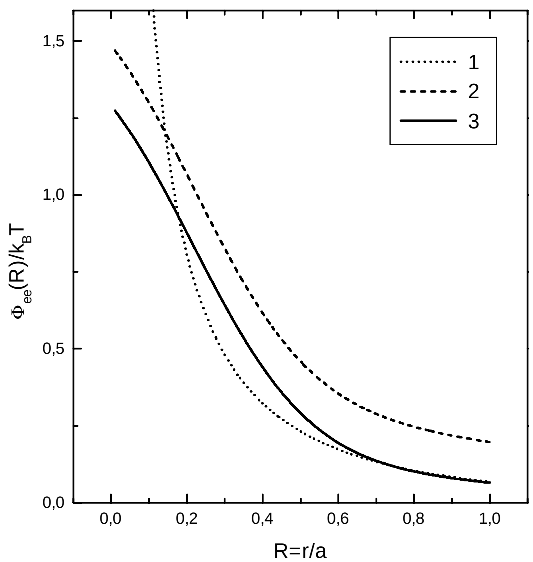

Fig. 1. Electron-electron pseudopotential of semiclassical hydrogen plasma against the dimensionless distance $R = r/a$ at $r_{\rm s} = 1.0$ and $\Gamma = 0.2$; 1: Debye-Hückel potential (13); 2: potential (5); 3: pseudopotential (11).

C. $\lambda_{\rm ii}, \lambda_{\rm ei}, \lambda_{\rm ee} \to 0$, $r_{\rm De}, r_{\rm Di} \to \infty$, then

$$\Phi_{\rm ab}(r) = \frac{e_{\rm a}e_{\rm b}}{r}\,. \quad (15)$$

In the absence of both quantum-mechanical effects and collective events, the pseudopotential $\Phi_{\rm ab}(r)$ coincides with the Coulomb potential.

D. $\lambda_{\rm ii}, \lambda_{\rm ei}, \lambda_{\rm ee} \ll r_{\rm Di}, r_{\rm De}$, then

$$\Phi_{\rm ab}(r) = \frac{e_{\rm a}e_{\rm b}}{r}\left[\exp\left(-\frac{r}{r_{\rm D}}\right) - \exp\left(-\frac{r}{\lambda_{\rm ab}}\right)\right] + \delta_{\rm ae}\delta_{\rm be}k_{\rm B}T\ln 2\exp\left(-\frac{r^2}{\lambda_{\rm ee}^2\pi\ln 2}\right). \quad (16)$$

This expression differs from the potential (5) with the presence of $\exp(-r/r_{\rm D})$ term in the brackets instead of 1. It corresponds to the weakly coupled plasma with $\Gamma \ll 1$.

In Figure 1 the electron-electron pseudopotential of semiclassical hydrogen plasma at $r_{\rm s} = 1$ and $\Gamma = 0.2$ is plotted. In the same figure we also show the potential (5) and the Debye-Hückel potential (13). As one can see the effective potential (11) coincides with Debye-Hückel potential at large distances and is as finite at the origin as the potential (5).

4 Radial distribution functions

It is well-known that the radial distribution functions are usually used to determine thermodynamic properties of various physical systems. They reproduce the probability density of discovering of one particle at the distance $\mathbf{r}$ from the other. To obtain them the variety of theoretical approaches is applied and among them the Bogolyubov method is a widely spread one. In the third section of this paper starting from the chain of Bogolyubov equations for the equilibrium distribution functions the procedure to derive the pseudopotential $\Phi_{\rm ab}(r)$ taking into account both quantum-mechanical effects of diffraction and symmetry and screening field effects has been described. In the pair correlation approximation the radial distribution function $g_{\rm ab}(r)$ of particles can be easily expressed through this effective potential:

$$g_{\rm ab}(r) = \exp\left(-\frac{\Phi_{\rm ab}(r)}{k_{\rm B}T}\right). \tag{17}$$

When Γ is not very large the radial distribution functions (like the pseudopotential $\Phi_{\rm ab}(r)$) have monotonic character. In this case expanding the exponent in formula (17) in weakly coupled regime and using (16), one can obtain the expression for radial distribution function which is rather analogous to the results of reference [1,14]

$$g_{\rm ab}(r) = 1 - \frac{e_{\rm a}e_{\rm b}}{rk_{\rm B}T}\left[\exp\left(-\frac{r}{r_{\rm D}}\right) - \exp\left(-\frac{r}{\lambda_{\rm ab}}\right)\right] - \delta_{\rm ae}\delta_{\rm be}\ln 2\exp\left(-\frac{r^2}{\lambda_{\rm ee}^2\pi\ln 2}\right). \tag{18}$$

When Γ increases, in the curve of radial distribution functions (17) local maxima and minima appear because of the short-range order formation. Such non-monotonic behaviour can occur when the Coulomb coupling parameter Γ is sufficiently large:

$$\Gamma \geq \frac{1}{2}\sqrt{\frac{\pi r_{\rm s}}{6}}. \tag{19}$$

As it follows from (19) if the dimensionless density parameter $r_{\rm s}$ is small enough, the short-range order formation can appear in the system even if $\Gamma < 1$. To demonstrate this property we plot Figure 2 where the electron-electron radial distribution function at $r_{\rm s} = 0.1$ and $\Gamma = 0.3$ is shown. In Figure 2 it can be seen that the electron-electron radial distribution function has two maxima. As a matter of fact it has a great number of maxima but the oscillatory amplitude vanishes quickly enough due to the screening effects. It should be noted that the short-range order formation is the result of competition between the quantum-mechanical effects and screening field ones when the scales of their action are comparable.

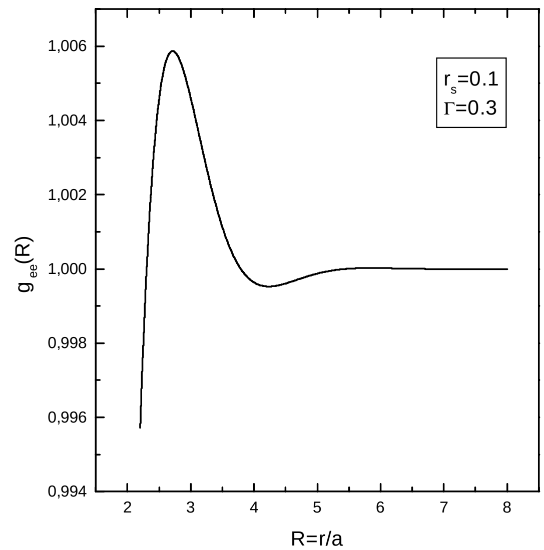

Fig. 2. Electron-electron radial distribution function of semi-classical hydrogen plasma against the dimensionless distance $R = r/a$ at $r_{\rm s} = 0.1$ and $\Gamma = 0.3$.

5 Correlation energy of plasma

One of the most essential thermodynamic characteristics determining plasma properties is an internal energy. Heat capacity, free energy and others thermodynamic potentials can be evaluated *via* it.

From the statistic theory of equilibrium state of systems consisting of the great number of particles it is well-known that the internal energy E can be written as follows

$$E = \frac{3}{2}Nk_{\rm B}T + U_N, \tag{20}$$

where N is a number of particles number in the system and correlation energy U_N is expressed *via* radial distribution functions $g_{\rm ab}(r)$ by means of

$$U_N = 2\pi V\int_0^\infty \sum_{\rm a,b} n_{\rm a}n_{\rm b}\varphi_{\rm ab}(r)g_{\rm ab}(r)r^2{\rm d}r, \tag{21}$$

here V is a volume of the system.

In case of small Γ the integration in formula (21) can be performed analytically with the aid of expression (18). Dropping the terms of $\lambda_{\rm ab}^2/r_{\rm D}^2$ order (they include quantum-mechanical effects of symmetry) one can obtain

$$U_N = -2\pi V\sum_{\rm a,b}\frac{n_{\rm a}n_{\rm b}e_{\rm a}^2e_{\rm b}^2}{k_{\rm B}T}r_{\rm D} + 3\pi V\sum_{\rm a,b}\frac{n_{\rm a}n_{\rm b}e_{\rm a}^2e_{\rm b}^2}{k_{\rm B}T}\lambda_{\rm ab}. \tag{22}$$

The first term in the expression (22) corresponds to the Debye-Hückel theory and the second one refers to the quantum ring sum or Montroll-Ward contribution [12]. As one would expect the weakening of interaction between charged particles due to the quantum effects of diffraction leads to the increase of plasma correlation energy.

In Figures 3 and 4 the correlation energy U_N of hydrogen plasma is presented against the Coulomb coupling parameter Γ at fixed $\theta = 10$ and $\theta = 5$. In these figures solid lines indicates the calculation *via* formula (21) with the

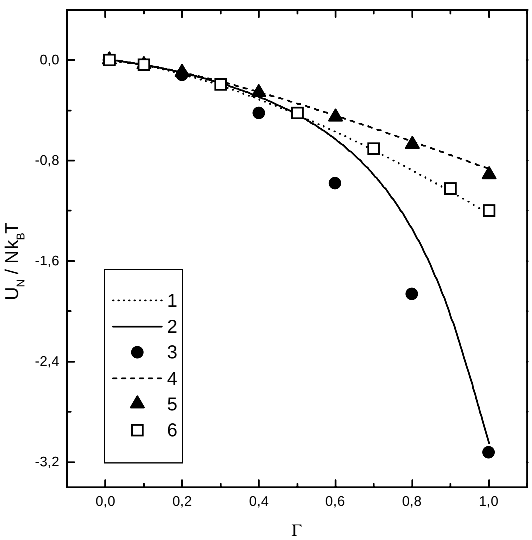

Fig. 3. Correlation energy of semiclassical hydrogen plasma against the dimensionless coupling parameter Γ at $\theta = 10$; 1: Debye-Hückel theory; 2: formula (21); 3: Tanaka *et al.* [13]; 4: formula (22); 5: Ichimaru *et al.* [21]; 6: Ebeling *et al.* [22].

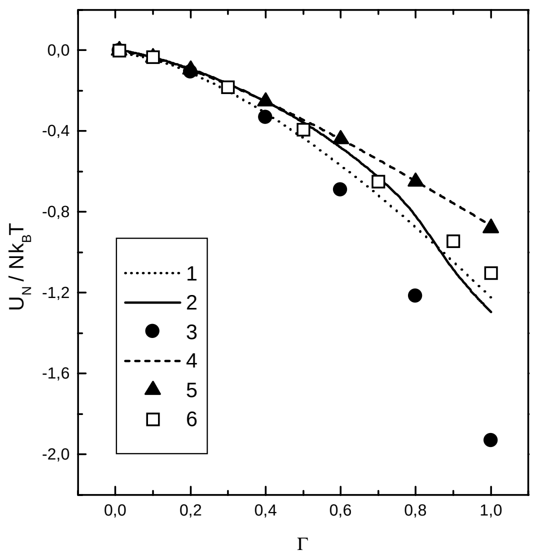

Fig. 4. Correlation energy of semiclassical hydrogen plasma against the dimensionless coupling parameter Γ at $\theta = 5$; 1: Debye-Hückel theory; 2: formula (21); 3: Tanaka *et al.* [13]; 4: formula (22); 5: Ichimaru *et al.* [21]; 6: Ebeling *et al.* [22].

use of the radial distribution functions (17); dashed lines represent the weakly coupled regime (22); dotted lines are the Debye-Hückel theory; solid triangles refers to the results of Tanaka *et al.* [13] where the density-response formalism with microfield correction was used; open squares indicate the data of Ebeling *et al.* [22] where on the basis of the available quantum-statistical results the Pade approximation of the correlation energy was performed; solid circles represent the results of Ichimaru *et al.* [21] where on the basis of the hypernetted-chain approximation the formation of bound states in plasma was taken into account.

In both figures it is not difficult to see that the data of Ebeling *et al.* [22] differs slightly from the Debye-Hückel theory because the degeneracy parameter θ is sufficiently large. For small Γ all theories confirm one another. The analytical formula (22) describes correctly the numerical calculations up to $\Gamma \sim 0.3$ and practically coincides with the results of [22] up to $\Gamma \sim 1$. As one would expect present data obtained with calculation *via* formula (21) as well as the results of Ichimaru *et al.* [21] lie lower than the other models. It is the result of contribution of bound states whose inclusion lead to the decrease of plasma correlation energy. It should be said that the inclusion of bound state effects in the above mentioned cases has been made in different ways. Ichimaru *et al.* [21] took into account formation of bound states by modified convolution approximation in the hypernetted-chain theory just as in the presented scheme bound state effects were included in the pseudopotential model (5) (see Refs. [16,17]).

When θ decreases, the correlation energy acquires a curve point (see Fig. 4). It is connected with the increase of role of quantum-mechanical effects of symmetry whose contribution is opposite to the contribution of quantum diffraction effects.

6 Conclusions

It is quite natural that the applied scheme has several restrictions. The first one is connected with the use of potential (5) at the derivation of which the formation of hydrogen molecules has been supposed to be prevented. It means that the plasma temperature must exceed 55 000 K. With the aid of the dimensionless parameters introduced in the second section this condition can be rewritten for hydrogen plasma in the form $\Gamma < 5.74/r_s$. The second restriction $\Gamma < 1$ appears due to the use of linearization process at the derivation of the integral-differential equation (6). In case of $\Gamma \geq 1$ effects beyond the pair correlation approximation must be accurately taken into account and that will be the subject of further investigations.

The main results of this paper can be itemized as follows:

(a) the inclusion of both quantum-mechanical effects and collective events in the pseudopotential of charged particles interaction leads to the screening effects at Debye radius-range distances and also to the finite quantity of the pseudopotential at the origin $r \to 0$;

(b) when plasma density increases, the short-range formation becomes possible even if the Coulomb coupling parameter is less than 1. It is the result of the competition between the quantum-mechanical effects and screening field ones when the scales of their action are comparable. This possibility is realized by means of that the electrostatic forces are screened, but the quantum interactions are not screened because they do not depend on number density of particles;

(c) the proposed pseudopotential model describes adequately the thermodynamic properties of dense high-temperature plasma in certain range of plasma parameters.

It should be noted here that on the basis of the proposed model not only thermodynamic but also transport properties of dense high-temperature plasma (such as electric conductivity and heat conduction) can be evaluated. Besides, when plasma density increases, the problem of inclusion of quantum-statistic effects (Fermi-Dirac distribution) arises. All above-mentioned will be the subject of the further investigations.

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