Quasi-classical Theory and Simulations of Hydrogen-like Quantum Plasmas

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Abstract

First the range of validity of a quasi-classical approach is analyzed and analytical formulae for the thermodynamical potentials are derived. Then a simple quasi-classical model for the quantum molecular dynamics of hydrogen-like plasmas is developed. The model is based on a quasi-classical wave packet representation and leads to effective momentum-dependent Hamiltonians. The quantum-mechanical effects corresponding to the Pauli and the Heisenberg principle are modeled by constraints in the Hamiltonian. Monte Carlo and Molecular Dynamics calculations are carried out for electron-, electron-positron-, and for hydrogen plasmas considering ensembles of 64 - 250 particles. A comparison with the analytical formulae shows reasonable agreement.

1 Introduction

The theory of hydrogen-like many particle systems belongs to the most difficult and fascinating problems of quantum statistics [1, 2, 3]. This is in particular connected with the appearance of a simple type of bound states. In dense plasmas beside the bound states other quantum effects connected e.g. with the Pauli exclusion and many particle collective effects appear [3, 4]. In the last time hydrogen-like systems attract much interest [5]. Several limiting cases were treated analytically [2, 3]. The quasi-classical approach led already in the sixties to the correct bound state contributions in the second virial coefficients [6]. Shortly after the complete quantum statistical expression for the second virial coefficient and the pair distribution function was obtained [7, 8, 9].

The analytical calculations mentioned so far cover only the limit of small densities. For this reason computer simulations of dense systems are of large interest. In particular we mention the Monte Carlo calculations developed by Ceperley and Alder [10] and several other workers [11, 12, 13, 14]. In the last time quasi-classical simulations of many-particle systems have received a great deal of interest because they are relatively simple and provide also informations on the microscopic dynamics. In particular we mention the semi-classical approach to the molecular dynamics of hydrogen-like systems developed by Klakow, Toepffer and Reinhard [15, 16]. In recent work we extended this approach to ionization phenomena [17, 18, 19]. We included also degeneracy effects by using momentum-dependent potentials [20, 21]. This approach follows a method developed by a series of authors as e.g. Wilets, Kirschbaum, Dorso and Randrup. Originally only the Pauli exclusion principle was simulated by a momentum-dependent two-body interaction [22, 23]. Later the Heisen-

berg effects were incorporated by another momentum-dependent contribution [24]. The hydrogen ground state was reproduced exactly, the ground states of H^-, He, Li, Ne and Ar were given better than 15%. Cohen applied this model to atoms with higher Z-values and derived reasonable results for the ground states of all atoms up to $Z = 38$ [25]. In general, the quasi-classical approach based on momentum-dependent potentials gives atomic energies being between Thomas-Fermi and Hartree-Fock calculations. The conclusion from the papers cited above is, that at least in some limitations quantum-mechanical effects and in particular the Heisenberg and the Pauli principles may be incorporated into a quasi-classical approach by using momentum-dependent potentials.

In this work we develop this approach but we do not consider extensions of the quasi-classical formalism by introducing specific quantum variables which lead to an extended phase space. This route is chosen in the so-called wave-packet dynamics which introduces the size and the speed of the spreading of the wave packet as additional variables [15, 16, 26]. As known this methods leads to several difficulties in formulating a statistical mechanics which are connected with unphysical excitations [15, 16, 19].

In our model the quasi-classical phase space has only 6 dimensions per particle. We will study first electron-positron plasmas which we consider as a model of greatest simplicity due to the mass-symmetry. These model systems show several cancellation effects which are connected with the high symmetry [29]. Then hydrogen plasmas with asymmetric masses are studied.

2 Analytical Theory in the Quasi-classical Approximation

We consider first the characteristic lengths and dimensionless parameters of the plasma: The average distance of the protons (electrons) is the Wigner-Seitz radius, $d = [3/4\pi n]^{1/3}$. Here $n = n_e = n_p$ is the density of protons (electrons) in the plasma. The Debye length is $r_D = 1/\kappa$ where $\kappa^2 = 8\pi n e^2$. The Landau length is defined by $l = e^2/kT$ and the Bohr radius which characterizes the ground state orbit is defined as $a_B = \hbar/mc^2$. The quantum effects connected with scattering states are described by the De Broglie wave-length of free electron motion $\Lambda = h/[2\pi mkT]^{1/2}$ and the De Broglie wave length of relative electron motion $\lambda = \hbar/[2\mu kT]^{1/2}$ where μ is the reduced electron mass. By means of these characteristic lengths we define the dimensionless parameter of the electron degeneracy $n\Lambda^3$ and the coupling parameter $\Gamma = l/d$ and the interaction parameter

$$\xi = \frac{l}{\lambda} = 2 \cdot (\frac{-E_0}{kT})^{1/2}. \tag{1}$$

where $E_0 = -\mu e^4/2\hbar$ is the ground state energy. The range of a quasi-classical approach is in principle given by the condition $\xi \geq 1$, i.e. the classical Landau length l should be large in comparison to the De Broglie length λ. Accordingly quasi-classical behavior is expected at low temperatures, This situation is quite opposite to that for van der Waals gases. Besides the condition that the temperatures are sufficiently low we have to require that the densities are not too large, i.e. the Bohr radius should be small in to the mean distance of the charges $a_B \leq d$. Altogether this leads to the two conditions of quasi-classicality

$$T \leq (-E_0)/k_B, n \leq a_B^{-3}. \tag{2}$$

Accordingly the quasi-classical region is a corner in the density-temperature plane.

The first successful quasi-classical approach to quantum plasmas was based on the method of Slater sums which are defined by the energy eigen values E_n and eigen functions Ψ_n

$$S(r_1, \cdots, r_N) = \text{const} \sum \exp\left(\frac{-E_n}{k_B T}\right) \left|\Psi_n\left(r_1, \cdots, r_N\right)\right|^2 \tag{3}$$

The quantum-statistical partition function and correspondingly also the free energy may be expressed as space integrals over the Slater sum as in the classical case [3]. The technique of Slater sums allows an easy access to the free energy and the distribution functions especially in the region of low densities. The Slater sums for Coulombic systems were studied first by Kelbg [30] and later in detail by several authors [3]. Kelbg developed a perturbation theory for the Slater sum of pairs of particles

$$S_2(r) = 1 \frac{+}{-} \frac{e^2}{kTr} \cdot F(\frac{r}{\lambda}) + O(\xi^2) \tag{4}$$

Here the $+$ corresponds to charges with opposite sign and $-$ to charges with equal sign. The thermal wavelength is defined by $\lambda = \hbar/\sqrt{mkT}$. The Kelbg function $F(x)$ reflects Heisenberg's quantum effects and is defined by

$$F(x) = 1 - \exp\left(x^2\right) + \sqrt{\pi}\,(x)\,(1 - \text{erf}\,(x)) \tag{5}$$

The expression $(e^2/r) \cdot F(r/\lambda)$ may be interpreted as an effective quantum-statistical potential which replaces the classical Coulomb potential. Kelbg's effective potential applies to the region of high temperatures. The quasi-classical approach to the Slater sums developed later in [6] was based on a quantum-mechanical treatment of the lower two-particle bound states and a classical

treatment of the higher bound states and the free states [6]. The result for the low-density free energy reads

$$F = F_i d - kTV \cdot \left(\frac{\kappa^3}{12\pi} \cdot \tau(\kappa a_q) - n^2 \cdot 8\pi^{3/2}\lambda^3 \cdot \sigma(T) + O(n^2 \cdot \hbar^3) + O(n^{5/2}) \right) \tag{6}$$

Here σ is the so-called BPL-partition function, where BPL stands for the names of the pioneers in that field Brillouin, Planck and Larkin:

$$\sigma(T) = \sum \left(\exp\left(\frac{-E_0}{kTs^2} \right) - 1 + \frac{E_0}{kTs^2} \right) \tag{7}$$

here s is the main quantum number. Further

$$\tau(x) = 1 - (3/4)x + (3/5)x^2 - \ldots \tag{8}$$

is the well-known Debye-Hückel function representing approximately the ring contributions and $a_q = \sqrt{\pi}\lambda/4$ [29]. In the quasi-classical limit the term $O(n^2 \cdot \hbar^3)$ does not appear what means, the that in the order n^2 the ring-contribution and the BPL-term are the only corrections to the limiting law [6]. Nowadays several terms completing the BPL-contribution are exactly known [3, 31]. Since the BPL-term contains $\hbar$ in the exponential, the quasi-classical limit should be carried out with some caution. In particular we mention that for low temperatures the exponent yields extremely large values what leads to problems with the convergence of density expansions. A more soft behavior shows the fugacity expansion, which is just an alternative way to represent the thermodynamic functions [1]. In the quasi-classical limit we obtain (up to the quadratic order) for the pressure the implicit equation

$$\beta p = 2 \cdot z + \frac{K^3}{12\pi} \cdot \tau(K a_q) + z^2 \cdot 8\pi\lambda^3 \cdot \sigma(T) \tag{9}$$

$$n = z + \frac{\beta e^2 K}{1 + K a_q} + z^2 \cdot 8\pi\lambda^3 \cdot \sigma(T) \tag{10}$$

Here z is the fugacity and

$$K^2 = 8\pi z e^2 \beta \tag{11}$$

This equation of state shows the correct limits at high temperatures $\beta p = 2n$ and at low temperatures $\beta p = n$. By comparison with the more complete quantum-statistical PACH approach [32] one can show that indeed the quasi-classical equation of state yields not only qualitatively correct results but even in quantitative respect rather good results. In particular this is true for mass-symmetrical systems i.e. for electron-positron plasmas. For later comparison with MD-results we need also the mean Coulombic energy density which is obtained from the pressure by derivation with respect to the interaction parameter e^2

$$u = -e^2 \frac{\partial}{\partial e^2} p = u_f + u_b \tag{12}$$

Here u_f is the contribution of the free states

$$u_f = -\frac{z e^2 K}{1 + K a_q} \tag{13}$$

and u_b is the contribution of the bound states

$$u_b = 16\pi\lambda^3 z^2 \sum_{s=1}^{\infty} (\beta E_s) \left[exp\left(-\beta E_s\right) - 1 \right] \qquad . \tag{14}$$

We note that $z = n^*$ may be identified with the density of the free electrons (positrons).

In this way the quasi-classical approach can be considered as a very reasonable approximation to the complete theory. From the physical point of view the basic content of the formulae given above is the semi-classical treatment of the free charges which includes contributions up to $\hbar^2$ and a full quantum treatment

of the bound states. This basic concept will be transferred now to the quantum molecular dynamics.

3 Wave Packet Dynamics for the Free Charges

In earlier work [21] a simple quasi-classical model of the quantum electron gas based on a quasi-classical dynamics with an effective momentum-dependent Hamiltonian was developed. Now this model will be extended to electron - positron plasmas. Due to the mass- and charge - symmetry these plasmas have much in common with the one-component electron plasma and furthermore many quantum effects cancel due to the mass symmetry (except for the bound state effects and the Pauli effects) [1, 3, 27, 29]. We consider the quasi-classical dynamics of a system of free electrons, free positrons and excitons (bound states) which are in thermodynamic equilibrium. The excitons (bound states) are not explicitly taken into account in the dynamics, they form a kind of a heat bath. The concentration of the neutral excitons is derived from the mass action law

$$n_0 = n^2 \cdot \Lambda^3 \sigma(T) \cdot \exp(-\mu_e x/kT) \tag{15}$$

where μ_{ex} is the excess part of the chemical potential of the (free) plasma (i.e. the difference between the full chemical potential and the Boltzmann contribution). This is equivalent to minimizing the free energy (neglecting charge-neutral interactions) at constant temperature or the internal energy at constant entropy [19].

Let us discuss now the quasi-classical dynamics of the free charges in our model. The quantum-mechanical effects corresponding to the Pauli and the Heisenberg principle are modeled by constraints in the Hamiltonian. For the

derivation of the effective interactions we use the concept of minimum uncertainty wave packets [19, 21]. The wave function corresponding to a minimum uncertainty wave packet (also denoted as a coherent state) are Gaussians:

$$\psi_o(x) = \text{const} \exp\left(-\frac{(x-q)^2}{2r_0^2} + \frac{ipx}{\hbar}\right) \tag{16}$$

Here r_0 is the mean dispersion of the wave function, which is a free parameter in this concept. The effective Hamiltonian is derived by averaging the original Hamilton operator with respect to antisymmetrized combinations of the test wave functions

$$H(q,p;\hbar) = \int d\mathbf{x} \psi_o^*(x) \hat{H} \psi_o(x) \tag{17}$$

From this expression one derives the following effective (quasi-classical) Hamiltonian

$$H(q,p;\hbar) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j} \delta_{ij} V_P\left(\frac{r_{ij}}{r_0}, \frac{p_{ij}}{p_0}\right) + \sum_{i<j} \frac{e_i e_j}{r} \cdot F\left(\frac{r_{ij}}{r_0}\right) \tag{18}$$

We have here two kinds of electron-electron and positron-positron interaction: the so-called Pauli-potential V_P, and a Coulomb interaction modified by a certain nonsingular function $F(x)$. The effective Hamiltonian $H(q,p;\hbar)$ is the generator of a Hamilton type phase space dynamics. Restricting the calculation described above to pair effects and averaging over the two spin configurations we get in some approximation for the direct term the KTR-potential [15]

$$F(x) = \frac{erf(x/\sqrt{2})}{x}, x = r/r_0, \tag{19}$$

and the Dorso - potential [22, 21]

$$V_P(p,r) = \frac{\hbar^2}{4mr_0^2} \cdot \exp\left\{-\frac{\Delta^2}{2}\right\} \tag{20}$$

This is an two-body interaction depending on the phase-space distance

$$\Delta^2 = \frac{p^2}{p_0^2} + \frac{r^2}{r_0^2} \tag{21}$$

with the minimum uncertainty condition

$$r_0 \cdot p_0 = \hbar \tag{22}$$

In the effective potentials r_0 is the width of the wave packets which we consider as a free parameter. Similar as in the Kelbg-potential we take for r_0 the thermal De Broglie wave-length $r_0 = \lambda/\sqrt{2} = \Lambda/2 * \sqrt{\pi}$ [19, 21].
On the basis of these potentials several Monte Carlo and Molecular Dynamics calculations were carried out for ensembles of 200 - 250 particles.

At first we carried out several runs for the OCP using the model described in [21]. The Coulombic part of the interaction energy per charge (in units kT) is given in Fig. 1 in comparison with the simple estimate

$$\epsilon^{OCP} = -\frac{e^2 K^{OCP}}{2(1 + K^{OCP} a_q)} \tag{23}$$

where $K^{OCP} = \sqrt{4\pi z e^2 \beta}$. Further a comparison with the Padé approximation from [28] and with DeWitt's formula fitting the classical MC-calculations [33]

$$\epsilon_{class}^{OCP}/kT = -0.896434\Gamma + 0.861856\Gamma^{1/4} - 0.5551 \tag{24}$$

is made. The results of our simulations for non-degenerate OCP ($\theta = 5$) and for weakly degenerate OCP ($\theta = 1, \theta = 2$) are well described by the quasi-classical estimate (23). For the case of degenerate OCP ($\theta = 0.15$) we get a better description by means of the Padé approximation given in [28]. At higher Γ-values ($\Gamma > 10$) the simulation-results for all investigated degrees of degeneracy θ are very near to the classical curve. This means the quantum effects are

rather small at $\Gamma > 10$ and we are unable to discriminate between the different theoretical estimates.

In a next step we calculated the energy density per particle for the two-component system (TCP) using the scaling rule

$$K^{OCP} \rightarrow K = \sqrt{2} K^{OCP} \tag{25}$$

We note that this simple scaling holds only for non-degenerate and weakly degenerate plasmas [29]. The results are given in Fig.2 in comparison with eqn.(13).

Further we carried out several simulations for the symmetrical TCP. The results are also given is Fig.2. For a given Γ-value the energies from the TCP-simulations increase with increasing degeneracy θ. The estimate (13) shows the same tendency, but there is no quantitative agreement. Further we see that the scaling rule (25) leads also to the same qualitative behavior. A more detailed comparison with Padé approximations, more accurate scaling rules and other simulation data is in preparation.

4 Superposition Representations of the Wave Packets

A disadvantage of the model described in the previous section is the approximate treatment of the bound states. Therefore we developed another approach, which is based on a superposition of free and bound electronic states. The free states are represented by Gaussian wave functions and the bound states by the 1s ground state wave function of the hydrogen atom. We restrict our consideration

to hydrogen, where the positive charges (protons) can be treated classically. Then the superposition ansatz reads [17]:

$$\Psi(x) = N_G \psi_G(x) + N_H \psi_H(x) \tag{26}$$

$$\psi_G(x) = (\pi r_0^2)^{-3/4} \cdot \exp\left(-\frac{(x-q)^2}{2r_0^2} + \frac{ipx}{\hbar}\right) \tag{27}$$

$$\psi_H(x) = (\pi a_0^3)^{-1/2} \cdot \exp\left(-\frac{|x-R|}{a_0}\right) \tag{28}$$

Here R denotes the position of the (next) proton. The parameters N_G and N_H may be considered as time-dependent variational parameters [17]. Here, we prefer another view where both parameters can only have the discrete values 0 or 1, i.e. an electron is either free or bound. In our molecular dynamics simulation, we consider stochastic transitions between both states, which leads to a dynamic equilibrium of ionization and recombination. A detailed description of this model can be found in [19]. We note that we have now two types of electrons in our system: free electrons with Gaussian wave functions and bound electrons with 1s-wave functions located at a nucleus. The effective interaction between free electrons remains unchanged. For the interaction between a free electron G and a bound electron H, we find

$$\begin{aligned} V_{GH} &= \frac{e^2}{r}\left\{\mathrm{erf}\left(\frac{r}{r_0}\right) - \frac{1}{2}e^{-r^2/r_0^2}\left[f\left(\frac{r_0}{a_0}+\frac{r}{r_0}\right) - f\left(\frac{r_0}{a_0}-\frac{r}{r_0}\right)\right]\right\} \quad , \\ & f(x) = e^{x^2}\,\mathrm{erfc}(x) \end{aligned} \tag{29}$$

Correspondingly, the interaction between two bound electrons reads

$$V_{HH} = \frac{\mathbf{e^2}}{a_0\rho} e^{-2\rho}\left[1 + \frac{5}{8}\rho - \frac{3}{4}\rho^2 - \frac{1}{6}\rho^3\right] \quad , \quad \rho = \frac{r}{a_0} \quad . \tag{30}$$

5 Formation of Molecules

The superposition ansatz describes in principle the formation of molecules. Let us consider a region of density and temperature where all electrons are in hydrogen states i.e. $N_G = 0, N_H = 1$. In this case, the dynamics of atoms is purely classical and the effective interactions are of Heitler-London type. Following the spirit of the Heitler-London theory we have to calculate the effective hydrogen-hydrogen interaction by taking into account the spins of the electrons explicitly. Assuming a system of electrons with 50% spin up and 50% spin down and considering symmetrized or antisymmetrized wave functions we obtain two effective potentials for the hydrogen-hydrogen interaction

$$V_{Hs} = \frac{Q + A}{1 + S^2} \tag{31}$$

$$V_{Ht} = \frac{Q - A}{1 - S^2} \tag{32}$$

where

$$Q = \frac{\mathbf{e^2}}{a_B \rho} e^{-2\rho} \left[1 + \frac{5}{8}\rho - \frac{3}{4}\rho^2 - \frac{1}{6}\rho^3 \right] \tag{33}$$

$$A = \frac{\mathbf{e^2}}{a_B} \left\{ \frac{S^2}{\rho} \left[1 + \frac{6}{5}(C + \ln \rho) \right] - e^{-2\rho} \left[\frac{11}{8} + \frac{103}{20}\rho + \frac{49}{15}\rho^2 + \frac{11}{15}\rho^3 \right] \right. \tag{34}$$

$$\left. + \frac{6M}{5\rho} \left[M \,\mathrm{Ei}(-4\rho) - 2S \,\mathrm{Ei}(-2\rho) \right] \right\} \tag{35}$$

$$S = \left(1 + \rho + \frac{1}{3}\rho^2 \right) e^{-\rho} \tag{36}$$

$$M = \left(1 - \rho + \frac{1}{3}\rho^2 \right) e^{\rho} \tag{37}$$

$$\rho = \frac{R}{a_B} \quad , \quad C = 0.57722 \quad , \quad Ei(x) = \int_{-\infty}^{x} \frac{e^t}{t} dt \tag{38}$$

$$\tag{39}$$

The singlet state with anti-parallel spins corresponds to a potential with a minimum at $R_0 = 1.6 a_B$ with a depth $V_{Hs}(R_0) = -3.2 eV$. This is of course only a

rough approximation of the real intra-atomic interactions. More realistic calculations give the figures $1.4a_B$ and $-4.4eV$. The triplet state with anti-parallel spins yields a repulsing potential.

We carried out several simulations with the potentials given above at different densities and temperatures. In nearly all cases we observed the formation of long chains of hydrogen atoms, alternatively with up and down spins. This is due to the fact that we neglected three and four particle interactions, which are essential for the description of atom-molecule and molecule-molecule interactions. In our simple model, the repulsion between two atoms in triplet states which are next to nearest in a chain are not strong enough to prevent the formation of chains. In order to avoid this false effect, we have made an artificial modification of the triplet-potential: We simply increased the strength of this potential (by about a factor two). As shown in Fig. 4 this model leads to more realistic description of the formation of molecules.

We have calculated also the pair correlation function of the atoms, which is shown in Fig. 5. The sharp maximum of $g(R)$ at a distance of about $1.6a_B$ reflects the atoms bound in molecular states.

6 Discussion

We started this work with a survey of the available results on the quantum statistics of hydrogen-like plasmas in quasi-classical approximation. Then we developed a simple quasi-classical model for the dynamics of hydrogen-like plasmas based on effective momentum-dependent Hamiltonians. The quantum-mechanical effects corresponding to the Pauli and the Heisenberg principle were by constraints in the Hamiltonian. By using the concept of minimum uncer-

tainty wave packets, momentum-dependent effective potentials were derived. The theory was applied first to electron-positron plasmas, which in some respect are the simplest possible case due to several cancellation effect. Then the theory was extended to a superposition model which represents the wave function as a sum of Gaussian and hydrogen 1s wave functions. Finally we studied the formation of molecules.

We simulated many-particles system with periodic boundary conditions by using Monte Carlo and Molecular Dynamics techniques. We considered ensembles of 64 - 250 particles. The main advantage of molecular dynamics simulations in comparison to Monte Carlo methods is that non-equilibrium properties are accessible. Of course, we cannot expect that the present model, which contains equilibrium parameters as the thermal De Broglie wave length will describe non-equilibrium properties in a quantitative way. Further improvements of the model might be unavoidable. Our strategy is a successive approximation were the correct representation of the known equilibrium and near equilibrium properties serves as a testing ground for the theory.

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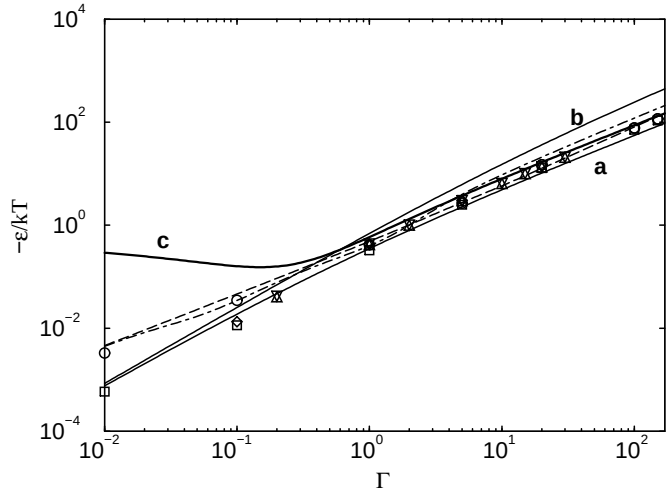

Figure 1: OCP - Interaction energy per particle in kT-units for $\theta = 0.15(\bigcirc)$, $\theta = 1.0(\square)$, $\theta = 2.0(\triangle)$, $\theta = 5.0(\triangledown)$. For comparison the curves from eqn. (23) (a: $\theta = 0.15$, b: $\theta = 5$), the Padé approximants [28] (dashed line: $\theta = 0.15$, dot-dashed line: $\theta = 5$) and the fit-formula (24) (c) are shown.

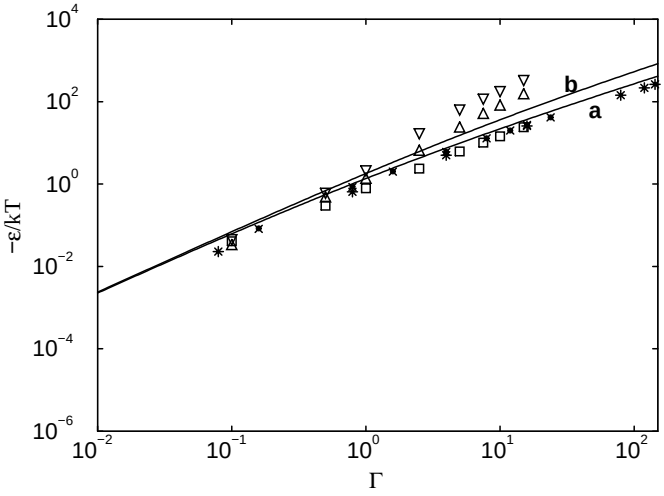

Figure 2: TCP - Interaction energy per particle in kT-units for $\theta = 1.0(\square)$, $\theta = 2.0(\triangle)$, $\theta = 5.0(\triangledown)$. In addition data from OCP simulations scaled according to the scaling rule (25) for $\theta = 1.6(*)$, $\theta = 3.2(\times)$, $\theta = 7.0(\bullet)$ is shown. The solid lines represent eqn. (13) (a: $\theta = 1$, b: $\theta = 5$)

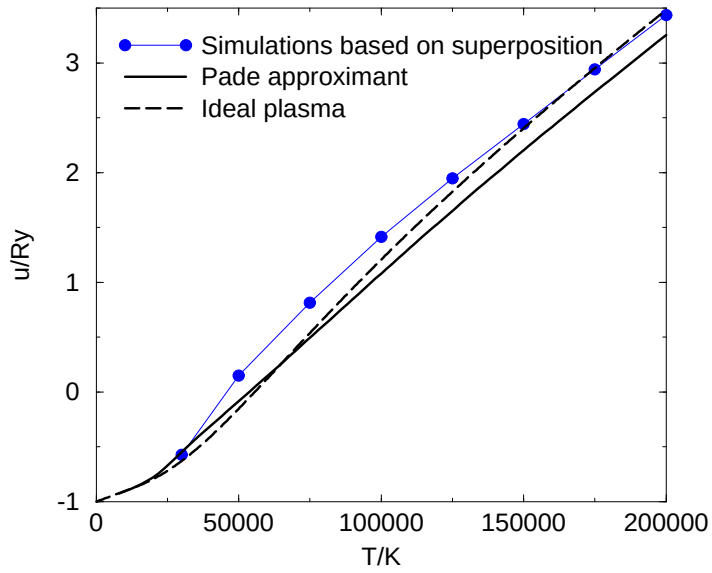

Figure 3: Internal energy of the hydrogen plasma at the density $n = 1.35 \times 10^{22}\, cm^{-3}$. Simulation data (•) are compared with the ideal plasma (dashed line) and the Padé approximant (solid line).

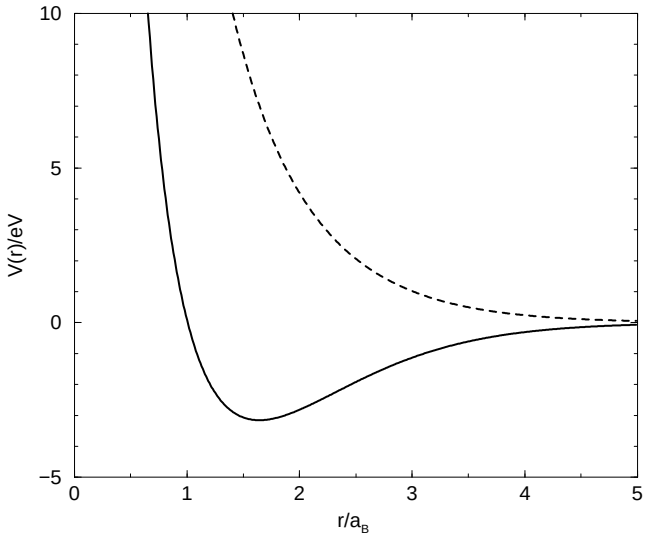

Figure 4: Potential of the effective interaction between two hydrogen atoms in the singulet-state (solid line) and the triplet state (dashed line).

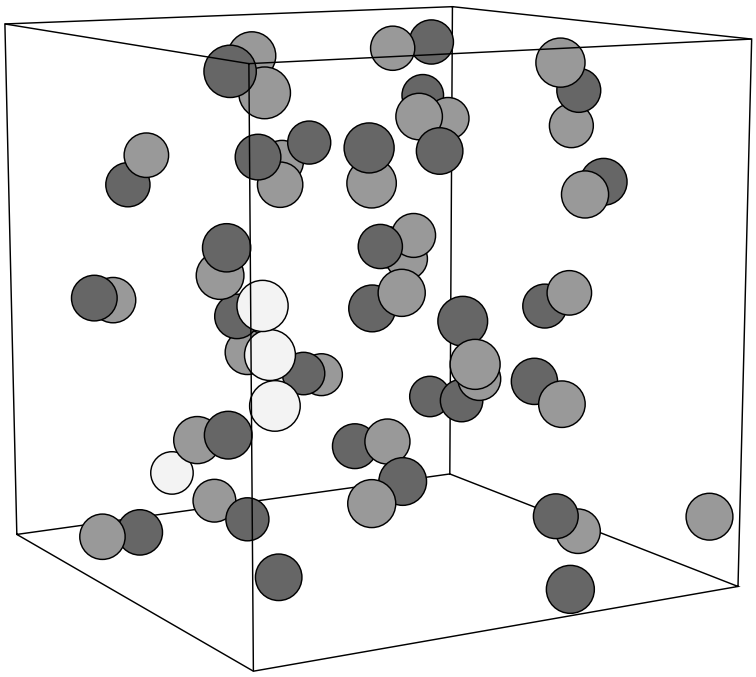

Figure 5: Formation of H_2 molecules at temperature $T = 300K$ and density $n = 6.75 \times 10^{22} cm^{-3}$. Atoms not bound in a molecule are colored white, bound atoms are colored dark-grey (spin up) and light-grey (spin down). Each molecule consists of one spin-up atom and one spin-down atom.

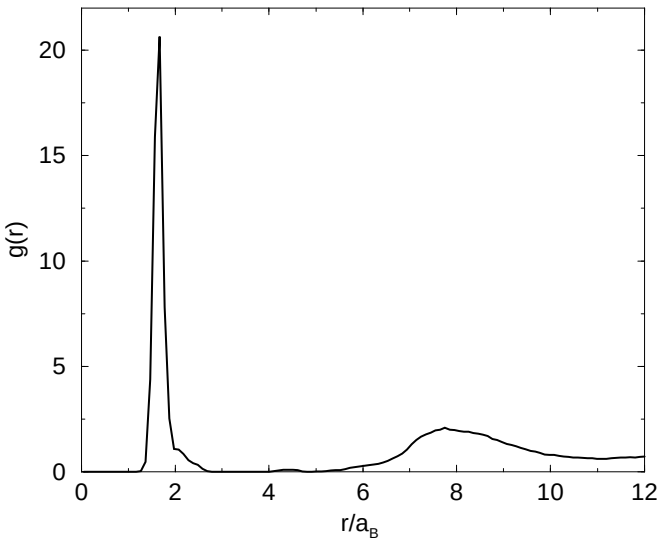

Figure 6: Pair correlation function of atoms. The peak at $R = 1.6a_B$ corresponds to the formation of H_2 molecules.