Classical 3-D Plasma Simulation Using CLAMPS Program

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1. Introduction

A central problem in plasma physics is to determine the equilibrium properties of a fully or partially ionized gas when the Coulomb particles are strongly interacting. In spite of the simple composition, hydrogen exhibits a surprisingly complex phase diagram, which is the subject of numerous experimental and theoretical approaches. In this project, we study the temperature regime of 100 K<T <11594 K where hydrogen undergoes a smooth transition with increasing temperature from a molecular fluid through an atomic regime and finally to a two component plasma of electrons and protons. In this project, we focus on low and intermediate densities 0.00019< r <0.5 g/cm^3 corresponding to 22>rs>1.5, where one expects the chemical models to work well although the properties of hydrogen are determined by the complex interplay of long-range Coulomb forces leading to strong

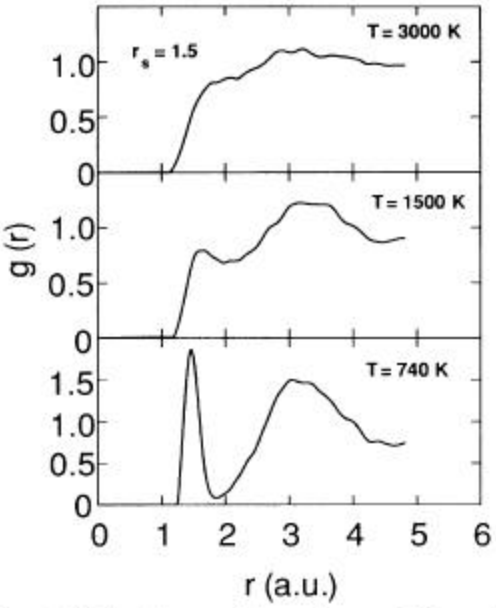

FIG. 2. $g(r)$ for the cooling phase of the simulation at r_s=1.5. Above ~1000 K $g(r)$ becomes increasingly featureless by overlap of intra- and inter-H_2 peaks (top and center) involving dissociation of molecules. Below 1000 K a strictly molecular phase is stable (bottom).

coupling and bound states as well as degeneracy effects.

In 1993, D. Hohl[2] did *ab initio* molecular dynamics simulations for high-density hydrogen (r_s=1.78-1.31, P=35-150GPa). Protons are treated as classical point charges and electrons in local density functional theory. The basic structural entity in this density

range is still hydrogen molecule but applying pressure changes the molecular ordering drastically. Molecules line up form filaments and eventually planes, where intermolecular distances become comparable to H_2 bond length. The phase diagram is strongly temperature dependent, and many different structures with very similar stability exist. The above figure shows how pair correlation function of the r_s=1.5 system changes with temperature. Starting the simulation from atomic initial structures, H_2 molecules form in the first few thousand MD steps with T<1000K. Increasing the temperature to 3000K the tow peaks merge.

In 2001, B.Militzer et. al. did restricted path integral Monte Carlo simulations to calculate the equilibrium properties of hydrogen in the density and temperature range of 9.8331024< r<0.153 g cm23 and 5000<T<250 000 K. They testes the accuracy of the pair density matrix and analyze the dependence on the system size, on the time step of the path integral, and on the type of nodal surface. They also characterized the state of hydrogen and describe the changes from a plasma to an atomic and molecular liquid by analyzing the pair correlation functions and estimating the number of atoms and molecules present.

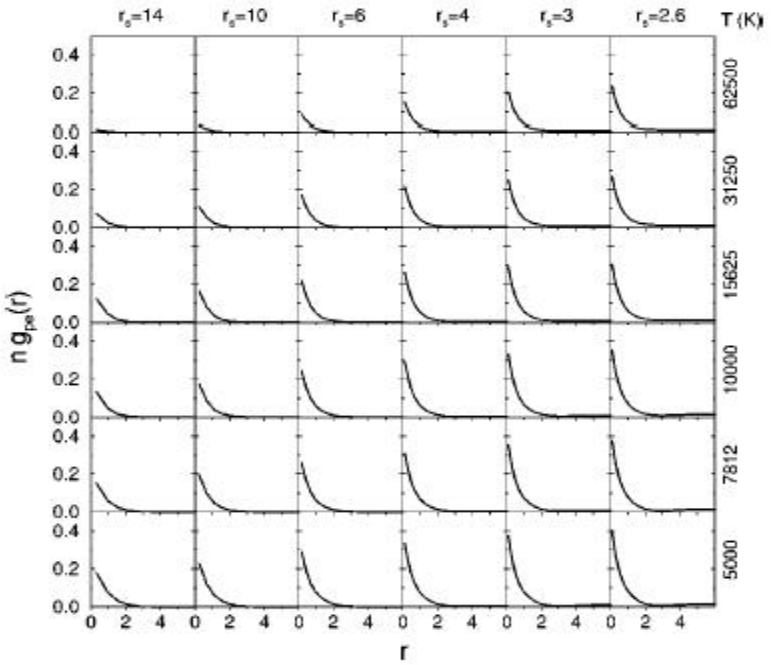

FIG. 17. Proton-electron pair correlation function multiplied by the density n. The columns correspond to different r_s values and the rows to different temperatures T.

The proton-electron pair correlation function multiplied by the density is shown in the above figure. The peak near the origin shows the increased probability of finding an electron near a proton due to the Coulomb attraction. The peak height decreases with temperature and increases with density because of thermal ionization and entropy ionization, respectively. At low temperature, the peak can be interpreted as occupation of bound states although ~unbound! scattering states can also contribute. From proton-electron pair correlation alone, one cannot distinguish between an atomic and a molecular state.

In our project, three kinds of pair correlation functions (proton-proton, electron-electron, proton-electron) are calculated using the results from the CLAMPS. Their implications to the phase diagram are discussed and the way we use CLAMPS is also included.

2. Input file for CLAMPS

To use CLAMPS, we must calculate the correct relationship amongst the input quantities so that energy=mass*(length/time)**2 and temperature is in units of energy.
In this project, we use electron volts for the units of energy and temperature, nanometer for length.
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✓ Density

The unit of density in the input file is the number of particles per nm^3. We shall also use a parameter the Wigner radius, given by

$$r_s = (3n_e / 4p)^{1/3}$$

where n_e is the mean electron density per unit volume. The density of hydrogen plasma we investigate range from 10^{-4} to $0.5\ g/cm^3$ ($1.5<r_s<20$).

✓ Potential

For the long range Coulomb potential:

$$V_c = \frac{q^2}{4pe_0 r}\,(\mathrm{J})$$

Thus, for interactions between protons and electrons, q should be

$$q = \left(\frac{1.6\times10^{-19}}{4pe_0 \times 10^{19}} \right)^{0.5} = 1.19945\,(eV^{1/2}/nm^{1/2})$$

To prevent protons and electrons recombine together, we add Yukawa potential, which is

$$V_Y = \frac{q^2}{4pe_0}\frac{e^{-r/r_D}}{r}$$

Where r_D is the plasma Debye length.

$$r_D = 750\left(\frac{Te(eV)}{n_e(cm^{-3})}\right)^{1/2} cm$$

For $r = 0.03 g/cm^3$, Te=0.025875eV (3000K), the Debye length is 0.0175 *nm*. Thus , the length scale for the Yukawa potential is

$$s = 1/r_D = 57.14$$

The energy scale is

$$\left(\frac{1.6\times10^{-19}}{4pe_0 r_D(nm)}\right)^{-1} = 0.00845$$

✓ Ewald Sum

To control the accuracy of the image potential for charged system, we define the distance in k space (number of k shells =*3*) at which to truncate the Fourier space coefficients for the Ewald sums and for which *S(k)* is computed.

We consider a system consisted by 16 protons and 16 electrons. For the case of r_s=*8, Te=0.2589eV* and 3 dimension problem , the input file is

```
DIMENSION 3
TYPE p 16 1 1.19945
TYPE e 16 0.001 -1.19945
POTENTIAL p p 2 1. 1. 0.672
POTENTIAL e e 2 1. 1. 0.672
POTENTIAL e p 2 1. 1. 0.672
POTENTIAL e p 4 57.14 0.00845 0.672
DENSITY 105.4
EWALD 3 1
TABLE_LENGTH 50000
TEMPERATURE 1.
LATTICE
SEED 10
WRITE_COORD 20
WRITE_SCALARS 20
RUN MC 20000 0.05
```

3. Simulation and Result Analysis

3.1 Adjustment of the size of the cube

The important parameter in Metropolis MC algorithm is the size of the cube used to generate trial positions. The length of one side is called d , and this is the last parameter in the input file that is entered into CLAMPS. Although it is not guaranteed that an acceptance ratio of 1/2 will optimize the simulation, usually we should adjust the value of d to make the acceptance ratio 1/2. Figure 1 shows the acceptance ratio as a function of d for the case of r_s=8, *Te=0.2589eV*.

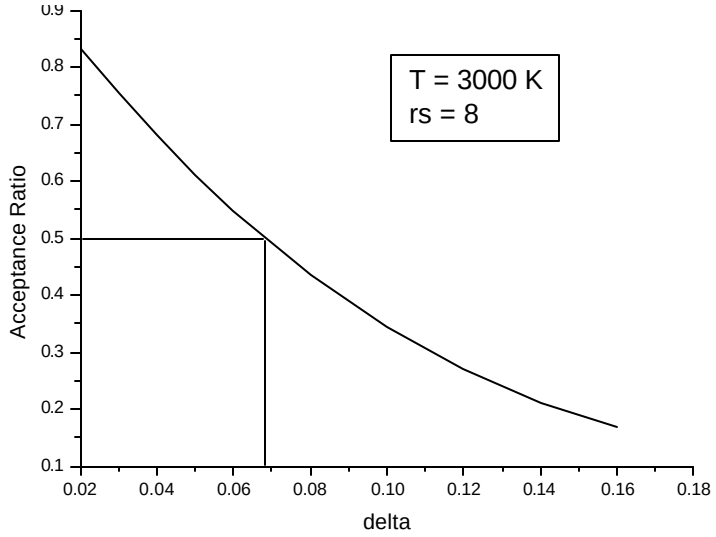

Figure.1. Tthe acceptance ratio as a function of d for the case of r_s=8, *Te=0.2589eV*

3.2 Results and Discussions

Simulations of two-component hydrogen plasma have been done using CLAMPS. There are three different pair correlation functions that can be directly obtained from many-body simulations and provide direct information about the state of the system. Shown in the following figures is an extensive set of pair correlations that allow one to estimate the microscopic structure of the system and allow a direct comparison with other simulations. The proton-proton pair correlation functions and proton-electron pair correlation functions from CLAMPS simulations are shown in Fig.2. and Fig.3. The cases for *rs=8.* rs=1.5 and rx=20 are shown in Fig.4 ~ Fig.7. For T=740K, rs=8, a peak at the r=0.21 nm($4a_0$)emerges, which clearly demonstrates the formation of hydrogen atoms. Started

from arbitrary positions, all particles pair up into H_2 molecules in 20000 steps. Those

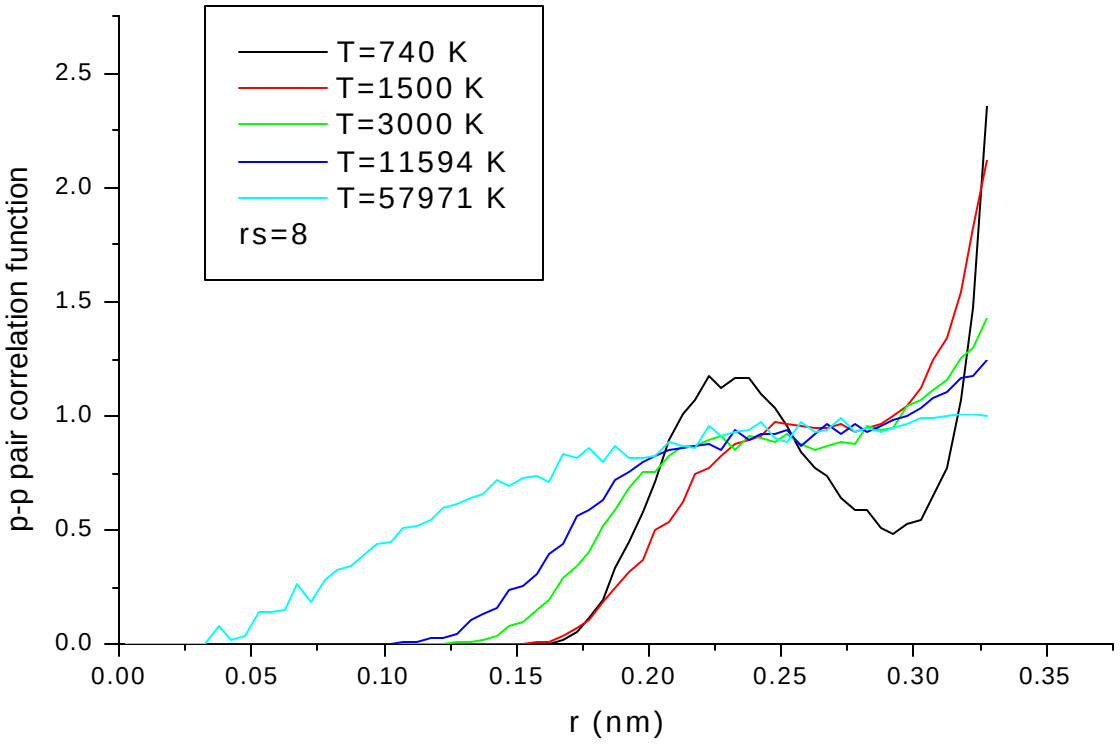

Figure.2. Proton-proton pair correlation function for different temperatures at rs=8

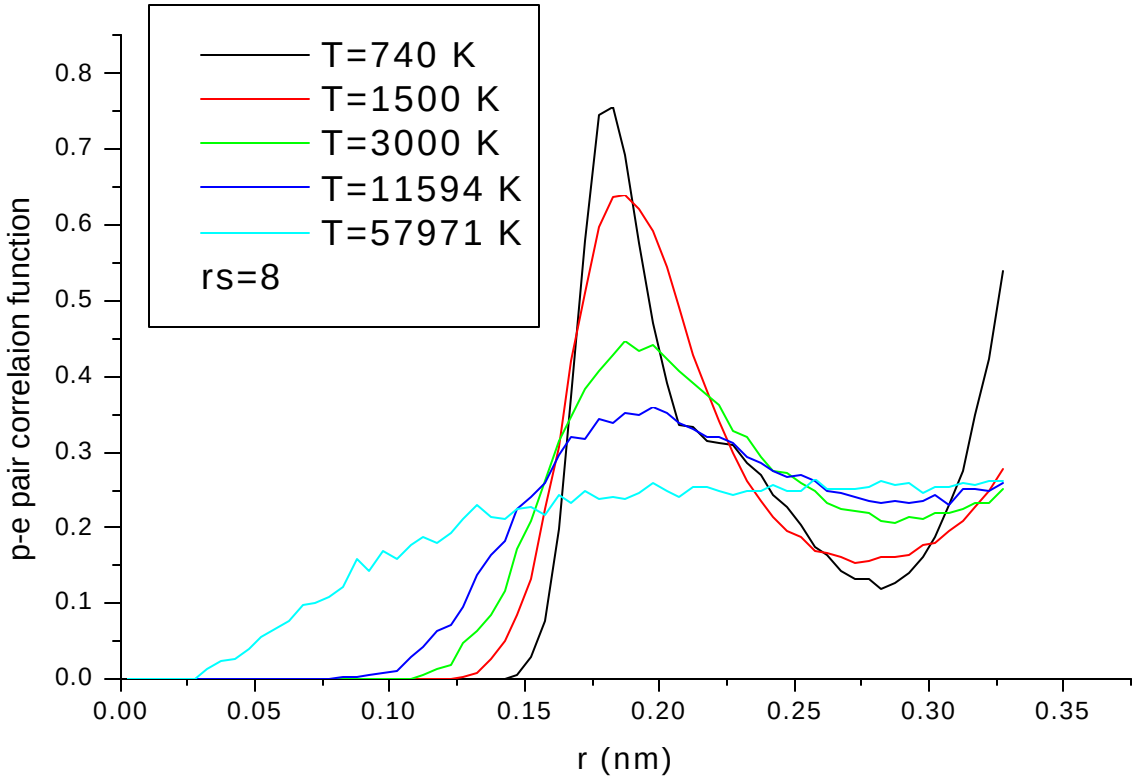

Figure.3. Proton-electron pair correlation function for different temperatures at rs=8

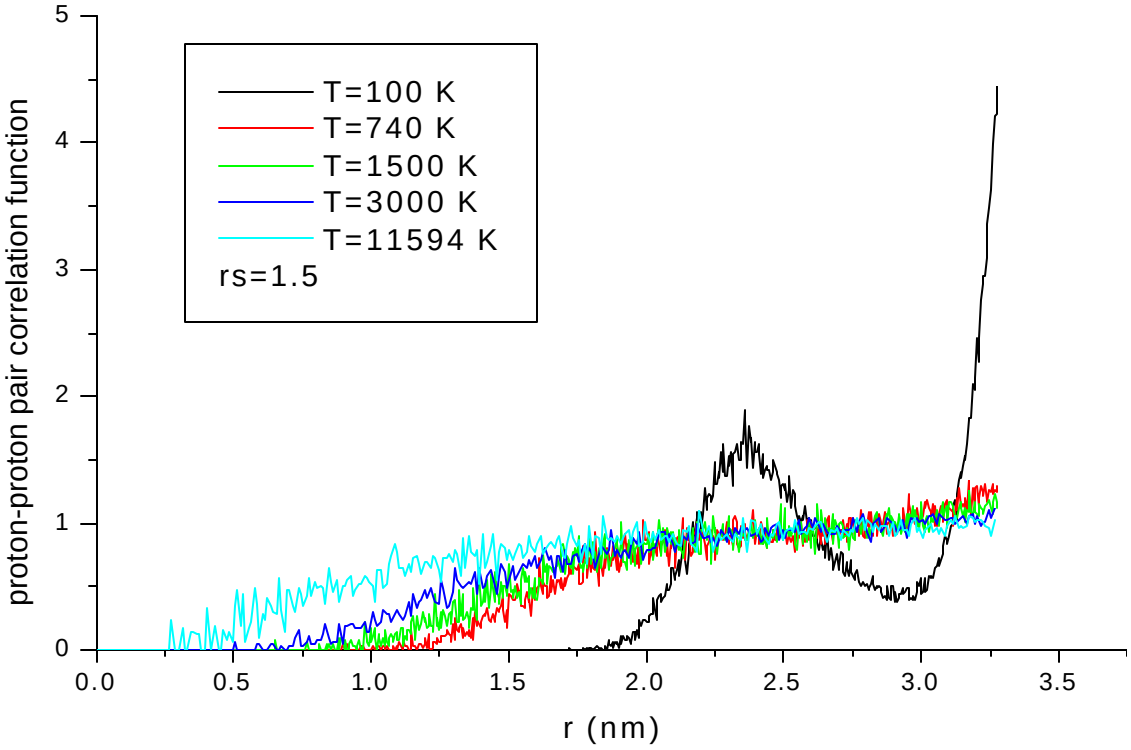

Figure.4. Proton-proton pair correlation function for different temperatures at rs=1.5.

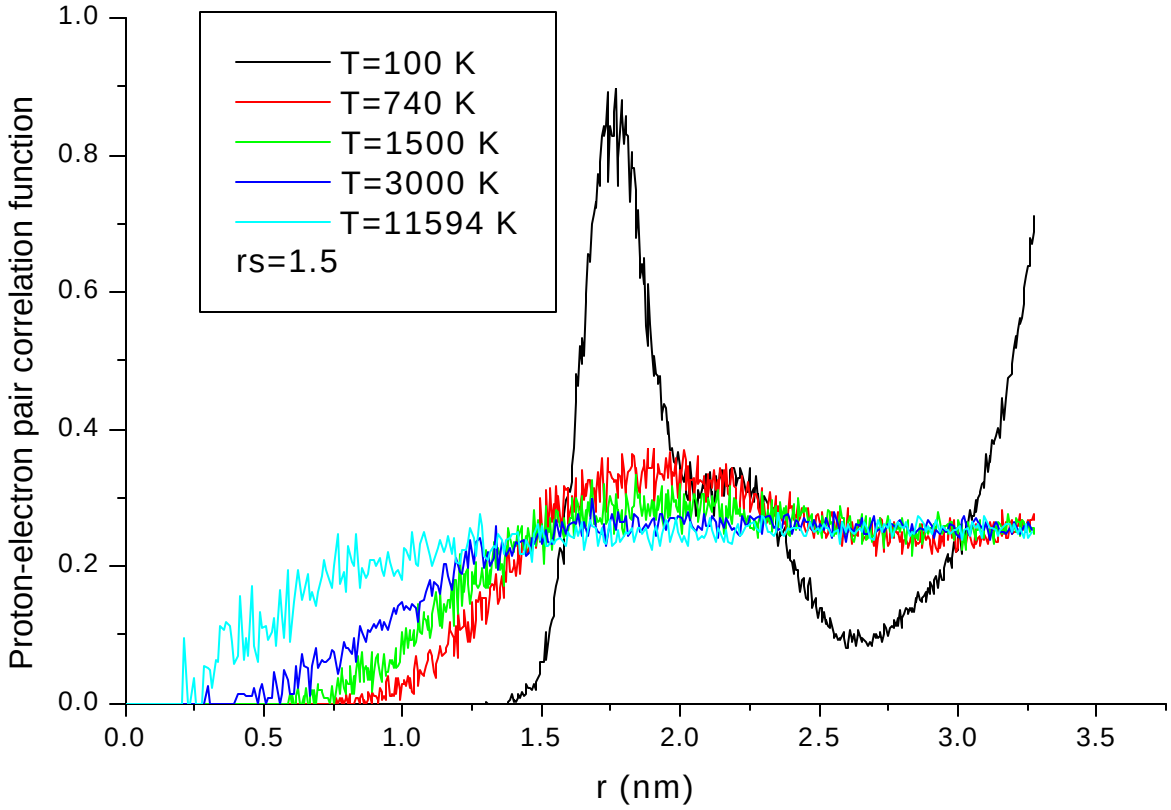

Figure.3. Proton-electron pair correlation function for different temperatures at rs=1.5

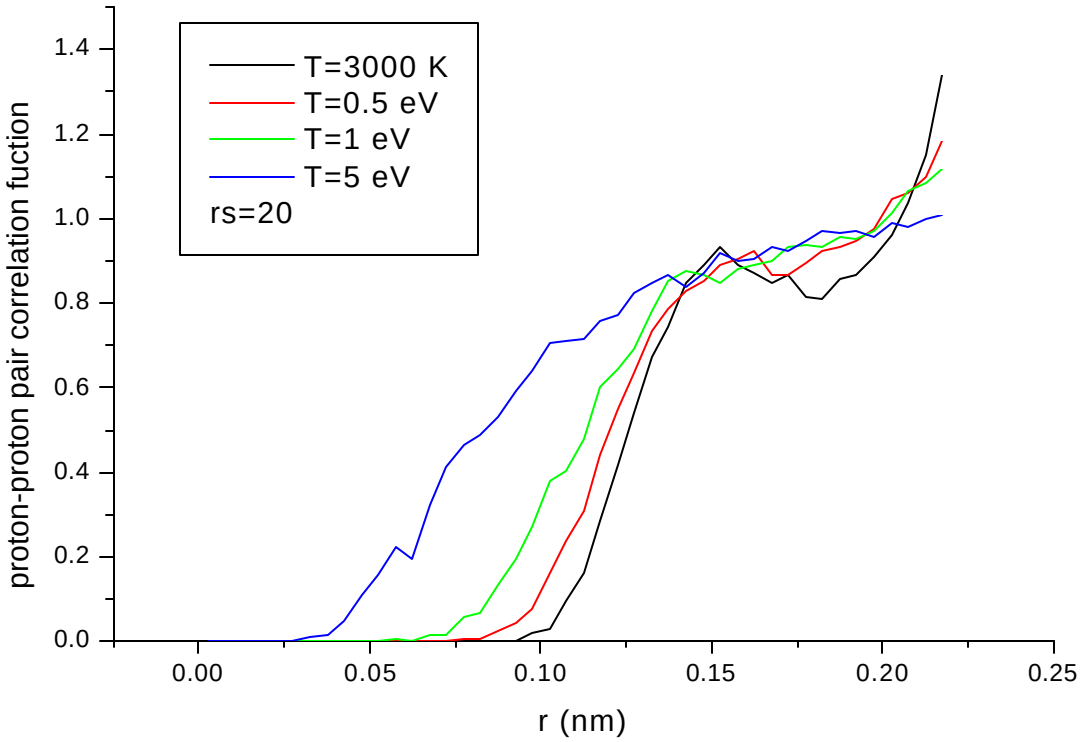

Figure.6. Proton-proton pair correlation function for different temperatures at rs=20

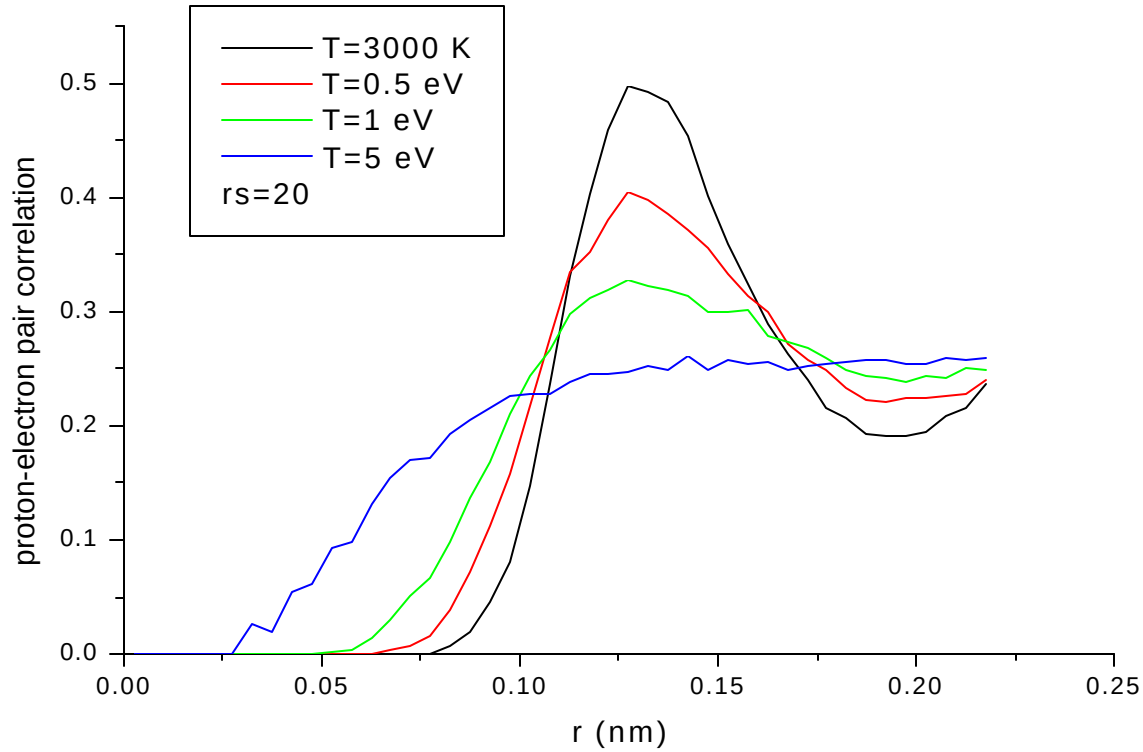

Figure.7. Proton-electron pair correlation function for different temperatures at rs=20

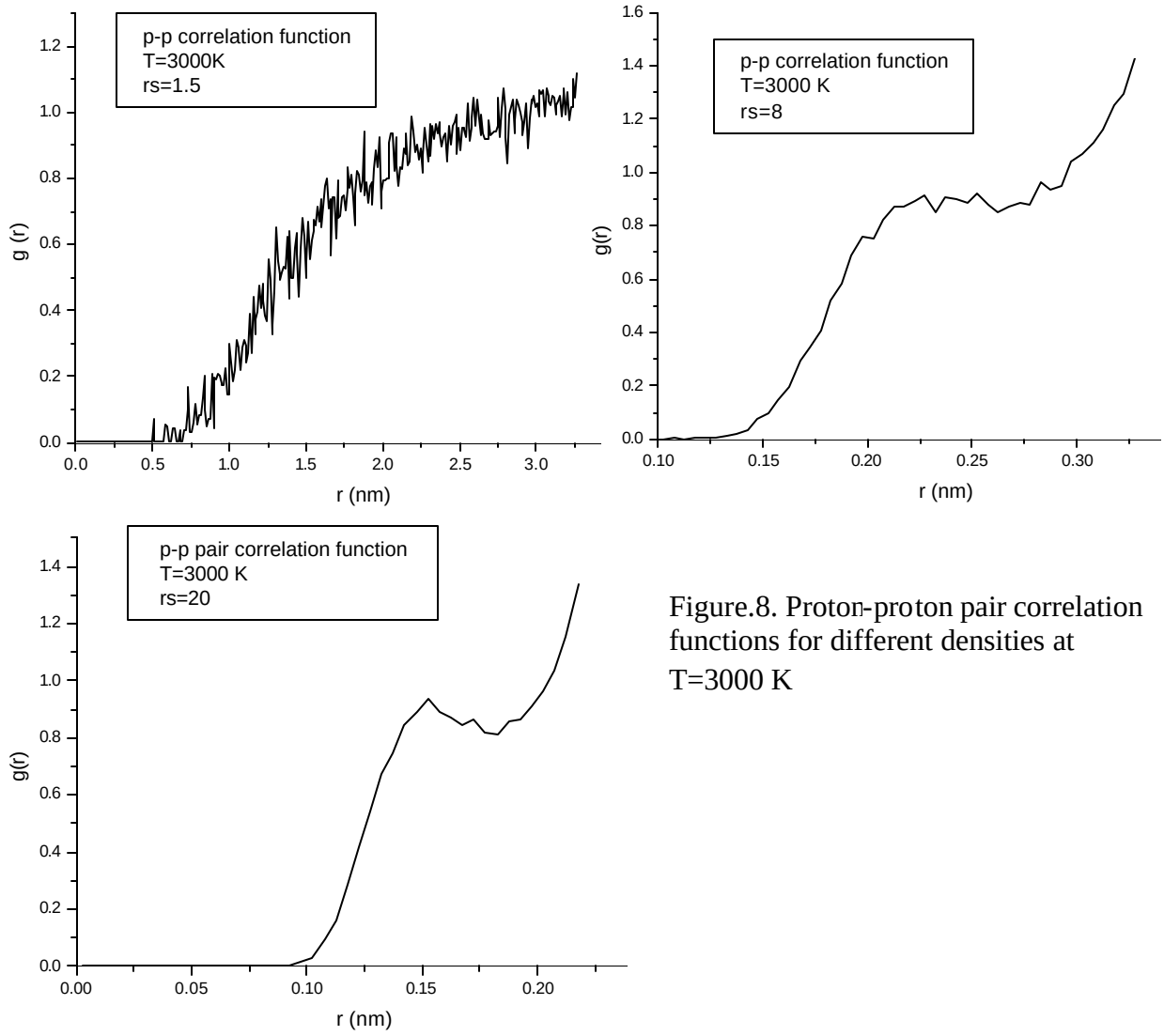

Figure.8. Proton-proton pair correlation functions for different densities at T=3000 K

figures shows that at T=57971 K the peak vanishes which means there is no atoms in the system and also demonstrate that at low densities and at sufficiently low temperature the plasma condenses into molecular hydrogen . At high densities, however, the condensation into both the molecular and atomic phases is suppressed by the strong interaction with the nearest neighbors. The peak height gets smaller with increasing temperature as a result of thermal and pressure ionization. At high temperatures (57971K), all systems are clearly in liquid states, while the individual particles diffuse but remain intact.

Increasing the density changes the picture. Fig.8. and Fig.9 shows that how the pair correlation function changes with density at fixed temperature T=3000 K. With increasing density, the proton-proton correlation first becomes broader and progressively

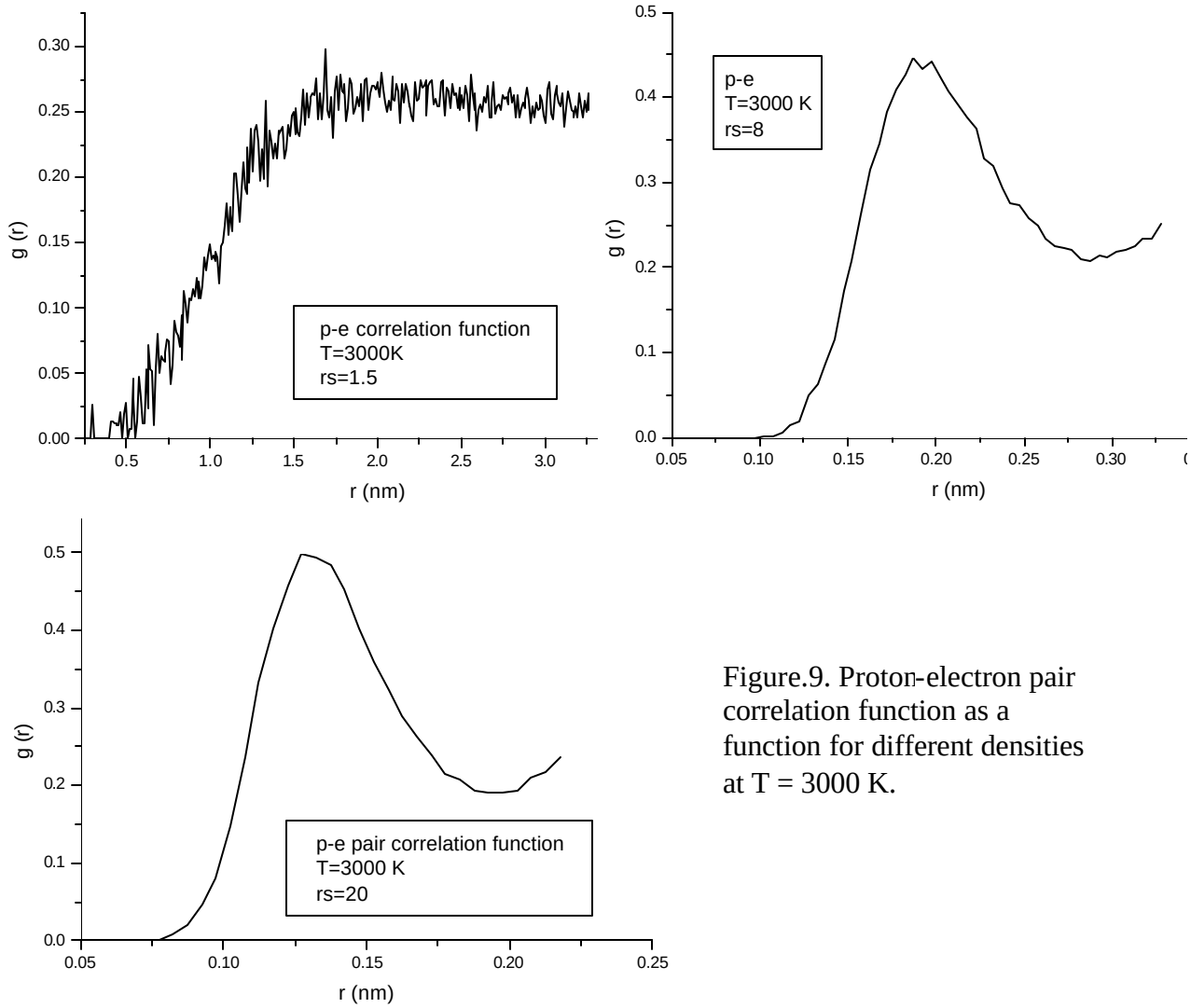

Figure.9. Proton-electron pair correlation function as a function for different densities at T = 3000 K.

more uniform. In Fig.9, as r_s decreases, pressure ionization occurs and the system is converted to fully ionized plasma.

4. Conclusions

In this work, we studied the high-temperature hydrogen plasmas at low and intermediate densities using MC method. The Metropolis MC scheme for the hydrogen plasma predicts essential features of the physical behavior of such a system—namely, the appearance or disappearance of atomic and molecular species as the temperature and density conditions are changed.

5. Thanks

We wish to thank Dr. Ceperley and Ken Esler for many detailed and valuable suggestions regarding this work.

References:

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