

Computer Simulation of Two Component Dense Plasma by Molecular Dynamics Method

Zh. A. Moldabekov* and T. S. Ramazanov

IETP, Al-Farabi Kazakh National University, 71 Al Farabi av., Almaty, 050040 Kazakhstan.

Received 14 March 2013; Accepted (in revised version) 24 May 2013

Communicated by Michel A. Van Hove

Available online 21 January 2014

Abstract. In the present work two component dense semiclassical plasma of protons and electrons is considered. Microscopic and electrodynamic properties of the plasma by molecular dynamic simulation are investigated. For these purposes semiclassical interparticle potential which takes into account quantum mechanical diffraction and symmetry effects is used. The considered range of density of plasma is $n = 10^{22} \text{cm}^{-3}$ to $n = 10^{24} \text{cm}^{-3}$. Fluctuations and dynamic dielectric functions were calculated using velocity autocorrelation functions.

AMS subject classifications: 81Q05, 82D10, 85A04

Key words: Molecular dynamic simulation, dense semiclassical plasma, semiclassical interparticle potential.

1 Introduction

At present dense plasma consisting of protons and electrons is a topic of intense investigation. First of all, the reason for this is the prevalence of hydrogen in the universe at present and in the past. For instance, inner matter of giant planets and stars (white dwarfs, brown dwarfs, the sun core) is a dense plasma. Furthermore, according to the Big Bang theory, up to 379 000 years after Big Bang protons and electrons dominated in the Universe. Consequently, understanding the properties of the dense plasma is very important for the investigation of the universe evolution. Secondly, in the ion beam and in the laser fusion experiments dense plasma is created and it is important to understand the processes in these experiments.

*Corresponding author. *Email address:* zhandos@physics.kz (Zh.A. Moldabekov)

The protons and electrons interact with each other via Coulomb potential

$$\phi_{Coulomb} = \frac{e_a e_b}{r_{ab}}, \quad (1.1)$$

where e_a, e_b are the charges of the particles and a, b are the types of the particles (proton, electron).

At short distance between particles the Coulomb potential tends to infinity. This problem can be solved by taking into account the quantum mechanical effects at short interparticle distance [1–7]. This has been achieved by approximating the Slater sum by a classical Boltzmann factor [8]:

$$S(r_1, \dots, r_N) = c \sum_n \Psi_n^* e^{-\beta E_n} \Psi_n, \quad (1.2)$$

where

$$c = \prod N_\nu! \lambda_\nu^{3N_\nu}, \quad (1.3)$$

$$\lambda_\nu^2 = 4\pi\alpha_\nu\beta, \quad \alpha_\nu = \hbar^2/2m_\nu, \quad \beta = 1/kT. \quad (1.4)$$

In these equations, N_ν is the number of particles of the ν -th species, which has mass m_ν and thermal wavelength λ_ν . The wave function is a properly symmetrized eigenfunction for the entire macroscopic system with eigenvalue E_n , where n represents a complete set of quantum numbers.

These are two types of quantum mechanical effects, the first one is the diffraction effect due to Heisenberg uncertainty and the second one is the symmetry effect due to Pauli exclusion principle. The second effect takes place for fermions.

Plasma properties can be studied by computer simulation, taking into account quantum effects in the interaction potential. For MD simulations, the following semiclassical interaction potential which takes into account quantum effects of diffraction and symmetry was used [8]:

$$\begin{aligned} \phi_{ab}(r) = \frac{e_a e_b}{r} \left\{ 1 - th \left(\frac{\lambda_{ab}^2}{a^2 + br^2} \right) \exp \left[-th \left(\frac{\lambda_{ab}^2}{a^2 + br^2} \right) \right] \right\} (1 - e^{-r/\lambda_{ab}}) \\ - \delta_{ae} \delta_{be} k_B T \ln \left(1 - \frac{1}{2} \exp \left(-\frac{r^2}{\lambda_{ee}^2} \right) \right), \end{aligned} \quad (1.5)$$

where $a = (4/3\pi n)^{-1/3}$ is the average interparticle distance, $b = 0.033$, $\lambda_{ab} = \frac{\hbar}{\sqrt{4\pi k_B m_{ab} T}}$ is the thermal wave length and $m_{ab} = m_a m_b / (m_a + m_b)$. The semiclassical interaction potential (1.5) was obtained using interpolation numerical data which were taken by numerical solving of the system of differential equations for the Fourier transform of the interaction potential in two component plasma [9]. In [9] Thomas-Fermi approximation was used for the determination of the wave function of the free particles. The ground-state wave function approximated by $\psi_G \approx \exp(-r/a)/\pi$. The method of calculating