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# Computer Simulation of Two Component Dense Plasma by Molecular Dynamics Method

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**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 $n=10^{22}cm^{-3}$ to $n=10^{24}cm^{-3}$. 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.

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The protons and electrons interact with each other via Coulomb potential

$$\phi_{Coulomb}=\frac{e_a e_b}{r_{ab}}, \tag{1.1}$$

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]:

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

where

$$c=\Pi N_\nu!\lambda_\nu^{3N_\nu}, \tag{1.3}$$

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

In these equations, $N_\nu$ is the number of particles of the $\nu$-th species, which has mass $m_\nu$ and thermal wavelength $\lambda_\upsilon$. 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]:

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

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

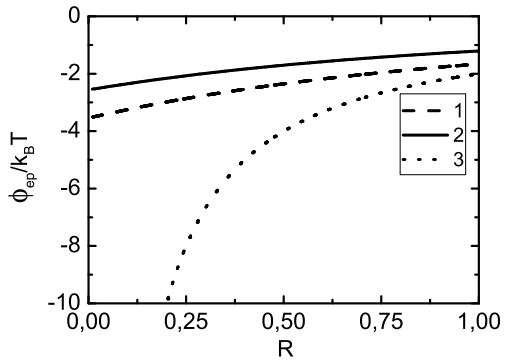


Figure 1: Proton-electron pair interaction potentials; 1 is the Deutsch potential, 2 is the semiclassical potential (1.5), 3 is the Coulomb potential. Here $R=r/a$, $\Gamma=2$, $r_S=1$.

the semiclassical potential presented in work [9] allows taking into account the influence of density effects on the diffraction term of the interaction potential. The diffraction term of the potential (1.5) at high temperature coincides with the potential of Deutsch $\phi_D(r)=e_a e_b(1-\exp(-r/\lambda))/r$ [10, 11]. The comparison of the semiclassical potential (1.5) with Coulomb and Deutsch potentials is shown in Fig. 1. It is seen that at short distances in a dense nonideal plasma the semiclassical potential (1.5) has lower absolute value than the Deutsch potential.

In the following, length is given in the terms of the average interparticle distance $a$, time is given in multiplies of the inverse of the plasma frequency $\omega_p=\sqrt{4\pi ne^2/m_e}$. Dimensionless parameters of plasma are coupling parameter $\Gamma=e^2/k_BTa$ and density parameter $r_S=a/a_B$, where $a_B$ is the first Bohr radius.

The standard molecular dynamics method [12–16] with periodic boundary conditions was used. In order to summarize the long range Coulomb interactions Evald procedure was utilized [17,18].

## 2 Microscopic properties

Microscopic properties of plasma can be investigated from analysis of the velocity autocorrelation functions, mean-square displacements of the velocity and coordinate. The velocity autocorrelation function is as follows:

$$K(t)=\left\langle \vec{\vartheta}(0)\vec{\vartheta}(t)\right\rangle=\frac{1}{3N}\sum_{i=1}^{N}\vec{\vartheta}_i(t_n)\vec{\vartheta}_i(t_n+t). \tag{2.1}$$

Mean-square displacement of any quantity $\chi$ can be obtained by the following formula

$$\left\langle \Delta\chi(t)^2\right\rangle=\frac{1}{N}\sum_{i=1}^{N}\Delta\chi_i^2. \tag{2.2}$$

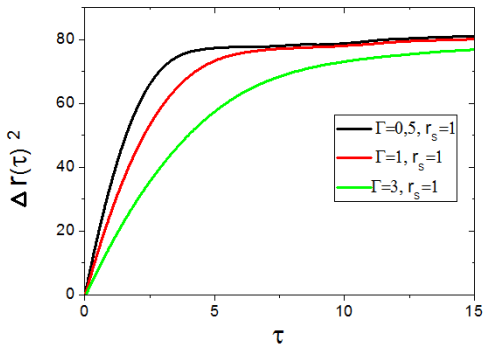


Figure 2: The mean-square displacements of the electron coordinates for several values of the coupling parameter at $r_S = 1$.

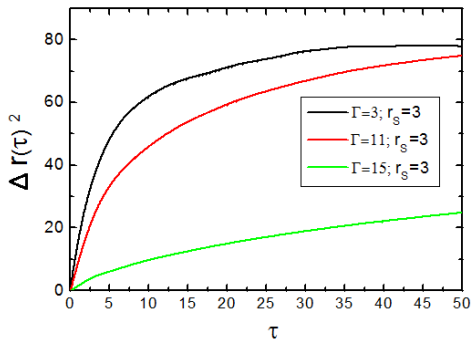


Figure 3: The mean-square displacements of the electron coordinates for several values of the coupling parameter at $r_S = 3$.

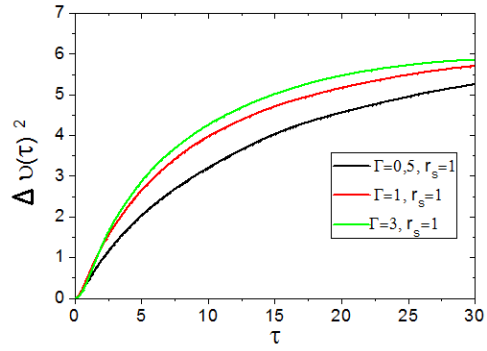


Figure 4: The mean-square displacements of the electrons velocity for several values of the coupling parameter at $r_S = 1$.

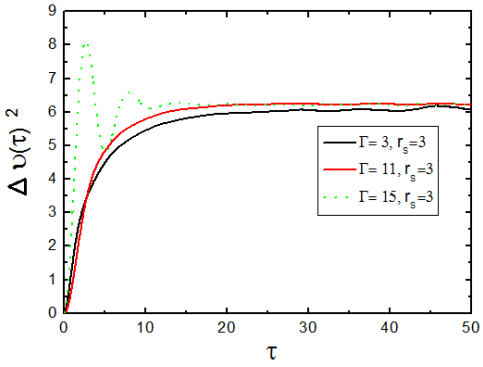


Figure 5: The mean-square displacements of the electrons velocity for several values of the coupling parameter at $r_S = 3$.

In Figs. 2 and 3 the mean-square displacements of the electron coordinates are shown. At initial time the electrons expand in the cell and the value of the mean-square displacement of the coordinates linearly increases. The mean-square displacement of the coordinates decreases with the increase of the coupling parameter (at fixed value of the density parameter) and of the temperature. Then, due to the limited size of the basic cell mean-square displacement of the coordinates tends to constant value. The same mechanism takes place for mean-square displacement of the electron velocity which is shown in Figs. 4 and 5.

The velocity autocorrelation functions calculated by the formula (2.1) are shown in Figs. 6-8. At a small coupling parameter the velocity autocorrelation function decreases monotonically with the increase in time. For a large coupling parameter the velocity autocorrelation function has an oscillating character. In the Fig. 9 the comparison of the velocity autocorrelation function obtained in present work using semiclassical potential

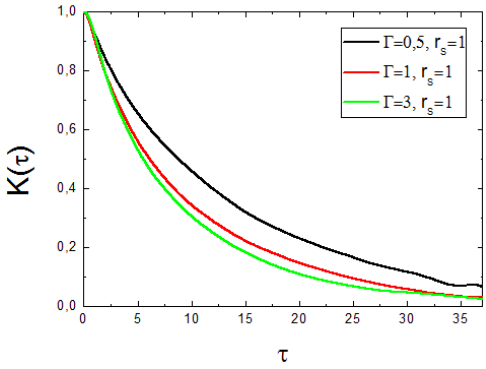


Figure 6: The velocity autocorrelation function of the electrons for several values of the coupling parameter at $r_S=1$.

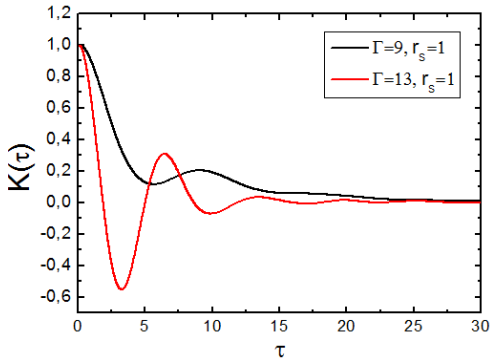


Figure 7: The velocity autocorrelation function of the electrons for several values of the coupling parameter at $r_S=1$.

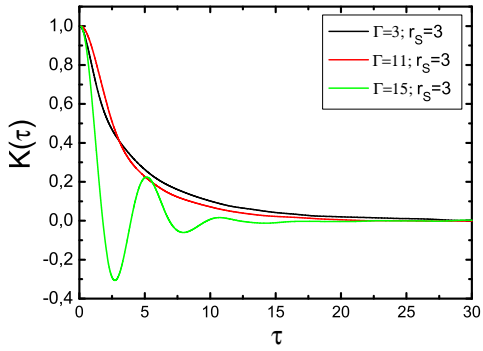


Figure 8: The velocity autocorrelation function of the electrons for several values of the coupling parameter at $r_S=3$.

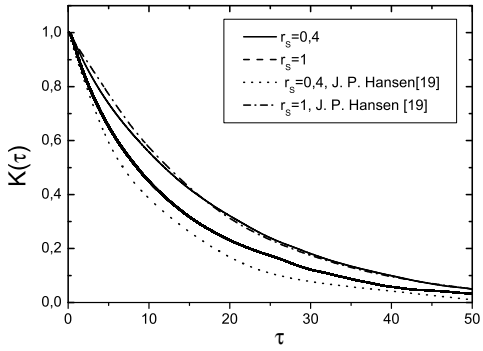


Figure 9: The velocity autocorrelation function of the electrons for several values of the density parameter at $\Gamma=0.5$.

(1.5) with the results of MD simulations of Hansen et al. [19, 20] based on the Deutsch potential is shown. It is seen that with increasing of density the difference between them increases due to increasing of the difference in magnitude between (1.5) and the Deutsch potential. The nature of the oscillations of the velocity autocorrelation function can be understood by spectral analysis of autocorrelation function. General susceptibility of plasma by the Fourier transform of velocity autocorrelation function has been obtained by the following formula [21]

$$\alpha(\omega)=\frac{e^2 n_e}{3k_B T}\int_0^\infty K(t)\exp(i\omega t)dt. \tag{2.3}$$

In the Figs. 10 and 11 real and imaginary parts of the general susceptibility for several plasma parameters are shown. Real part of the general susceptibility describes fluctuations in plasma while imaginary part is responsible for energy dissipation in plasma. At large coupling parameter real part has maximum when dimensionless frequency is

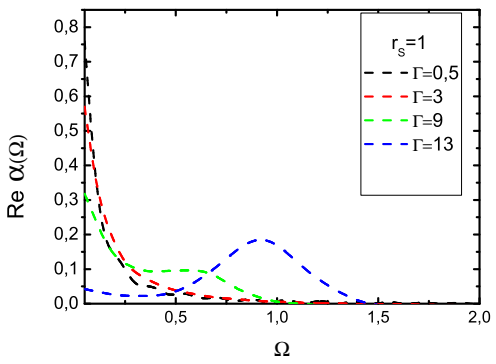


Figure 10: The real part of the general susceptibility for several values of the coupling parameter at $r_S = 1$.

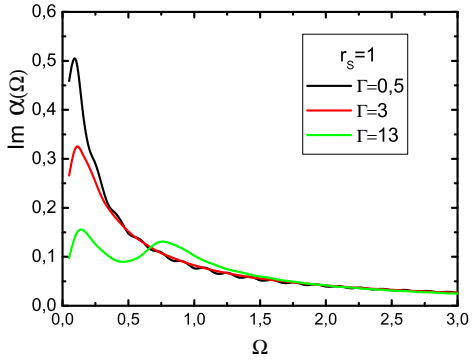


Figure 11: The imaginary part of the general susceptibility for several values of the coupling parameter at $r_S = 1$.

approximately equal to one. Physically, this means that in dense plasmas, Langmuir-like oscillations can appear at frequency $\omega_{Le} = \sqrt{4\pi n e^2/m_e}$.

From Fig. 11 of the imaginary part of the general susceptibility one can see that the waves with frequency less than Langmuir frequency should be strongly damping due to energy dissipation.

Dynamic dielectric function was calculated from

$$\varepsilon(\omega) = \left[1 - i\frac{4\pi\alpha(\omega)}{\omega}\right]^{-1}. \tag{2.4}$$

From Eq. (2.4) for the real part of the dynamic dielectric function we have:

$$\varepsilon(\omega) = \frac{1 + \frac{4\pi Im\alpha(\omega)}{\omega}}{\left(1 + \frac{4\pi Im\alpha(\omega)}{\omega}\right)^2 + \left(\frac{4\pi Re\alpha(\omega)}{\omega}\right)^2}. \tag{2.5}$$

Perturbation theory yields the well-known asymptotic $\omega \to \infty$ limit:

$$\varepsilon(\omega) = 1 - \frac{\omega_{Le}^2}{\omega^2}. \tag{2.6}$$

The real part of the dynamic dielectric function is shown in Fig. 12. The real part of dynamic dielectric function is characterized by a correct asymptotical behavior.

## 3 Conclusion

MD simulation of two component dense plasma with interparticle interaction potential which takes into account quantum mechanical effects has been fulfilled. It has been shown that in strongly coupled semiclassical plasma the waves with frequency less that

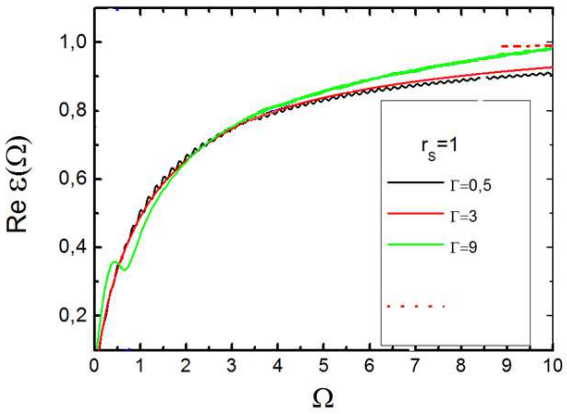


Figure 12: The real part of the dynamic dielectric function for several values of the coupling parameter at $r_S=1$. Red dot line is curve obtained from asymptotical formula (2.6).

Langmuir frequency are strongly damped similarly to those in weakly coupled plasma. It was found that at large values of coupling parameters in dense plasma, the Langmuir oscillations can be produced. It has been shown that semiclassical potential (1.5) correctly describes the properties of dense semiclassical plasmas.

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### References

[1] C. Deutsch, G. Maynard, M. Chabot, D. Gardes, S. Della-Negra, R. Bimbot, M. Rivet, C. Fleurier, C. Couillaud, D. Hoffmann, H. Wahl, K. Weyrich, J. Rosme, N. Tahir, J. Jacoby, M. Ogawa, Y. Oguri, J. Hasegawa, B. Sharkov, A. Golubev, A. Fertman, V. Fortov, and V. Mintsev, The Open Plasma Physics Journal, 3, 88 (2010).
[2] H. Nersisyan and C.Deutsch, Laser And Particle Beams, 29, 389 (2011).
[3] F.B. Baimbetov, M.A. Bekenov, and T.S. Ramazanov, Phys. Lett. A, 197, 157 (1995).
[4] W. Ebeling, G. Kelbg, and R. Sandig, Beitr. Plasma Phys., 10, 507 (1970).
[5] T.S. Ramazanov, K.N. Dzhumagulova, and Yu.A. Omarbakiyeva, Phys. Plasmas, 12, 092702 (2005).
[6] T.S. Ramazanov and K.N. Dzhumagulova, Phys. Plasmas, 9, 3758 (2002).
[7] F.B. Baimbetov, K.T. Nurekenov, and T.S. Ramazanov, Physica A, 226, 181 (1996).
[8] Zh.A. Moldabekov, T.S. Ramazanov, and K.N. Dzhumagulova, Contrib. Plasma Phys., 52, 207 (2012).
[9] M.A. Pokrant, A.A Broyles, and T. Dunn, Phys. Rev. A, 10, 379 (1974).
[10] C. Deutsch, Phys. Lett., 60 A, 317 (1977).
[11] C. Deutsch, Phys. Lett., 66 A, 381 (1978).

[12] J.M. Thijssen, Computational Physiscs (Cambridge University Press, New York, 2007).
[13] C. Wang, X.-T. He and P. Zhang, Commun. Comput. Phys., 12(4), 1121 (2012).
[14] T.S.Ramazanov, G.N. Nigmetova, G. Ropke, and R. Redmer, J. Plasma Phys., 72, 1031 (2006).
[15] F.B. Baimbetov, T.S. Ramazanov, K.N. Dzhumagulova et al., J. Phys. A: Math. Gen., 39, 4521 (2006).
[16] T.S. Ramazanov and K.N. Dzhumagulova, Contrib. Plasma Phys., 48, 357 (2008).
[17] P. Ewald, Ann. Phys. (Leipzig), 369, 253 (1921).
[18] D. Parry, Surf. Sci., 49, 433 (1975).
[19] J.P. Hansen et al., Phys. Rev. A, 23, 2041 (1981).
[20] J.P. Hansen et al., Phys. Rev. A, 24, 1544 (1981).
[21] F.B. Baimbetov and T.S.Ramazanov, High Temperature, 31, 786 (1993).