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Molecular dynamic simulation of the microscopic properties and electrical conductivity of a dense semiclassical plasma

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Abstract. The microscopic properties and the electrical conductivity of a dense semiclassical plasma are calculated by the molecular dynamics simulation method.

1. Introduction

In the present work we consider a fully ionized, strongly coupled (dense), semiclassical hydrogen plasma which occurs in astrophysical objects (interiors of white dwarfs, neutron star crusts, giant planets, etc.) and inertial fusion. The number density of particles is considered in the range $n = n_e = n_i \cong (10^{22} - 2 \times 10^{26})\,\mathrm{cm}^{-3}$, and the temperature domain is $T \cong (5 \times 10^4 - 10^6)K$. The following dimensionless parameters are used for the description of the system: the coupling parameter $\Gamma = e^2/ak_BT$, the density parameter $r_s = a/a_B$, and the time scale $t^* = t\omega_e$, where $\omega_e = (4\pi ne^2/m_e)^{1/2}$ is the electron plasma frequency. The degeneracy parameter is defined by the ratio of the thermal energy to the Fermi energy: $\Theta = k_BT/E_F \approx 0,54r_s/\Gamma$. Here e, a, a_B, E_F are the electrical charge, the Wigner–Seitz radius, the Bohr radius and the Fermi energy, respectively. The transport properties of non-ideal plasma can be studied by means of various theoretical methods, e.g. using path integrals, integral equation methods, kinetic equations, virial expansions, etc. Usually these methods are applied for coupling parameters $\Gamma \ll 1$ (weakly coupled plasma) and for $\Gamma > 100$ (strongly coupled, fully degenerate plasma). In the intermediate region between these limiting cases the transport properties of strongly coupled plasma can be studied by means of computer simulations, e.g. molecular dynamics [1–3].

2. Models for the interaction between the particles

In this work we use an effective semiclassical potential [4]. This potential contains quantum diffraction and symmetry effects [5, 6] at short distances and has a limiting value for $R \to 0$. At large distances it takes into account many-particle screening effects [7] and is strongly screened. With an increasing plasma density, the higher-order many-particle correlations have to be taken into account. In

this connection, the classical effective potential that accounts for three-particle correlations and the semiclassical effective potential that accounts for short-range quantum diffraction and symmetry effects as well as the long-range screening effects are used in this work. In the case of a three-particle approximation, the expression for the effective potential for a dense classical plasma is [7]:

$$\Psi(R) = \frac{\gamma}{R} e^{-R} \frac{1 + \gamma * f(R)/2}{1 + c(\gamma)}, \tag{2.1}$$

where $f(R) = [\exp(-\sqrt{\gamma}R) - 1]\,[1 - \exp(-2R)]\,/5$, $c(\gamma)$ is the correction coefficient; $\gamma = e^2/(r_{\mathrm{D}} k_{\mathrm{B}} T)$, γ is the parameter of non-ideality; $R = r/r_{\mathrm{D}}$; r_{D} is the Debye screening radius. The quantum mechanical diffraction and symmetry effects can be accounted for by the effective potential [5, 6]:

$$U_{\alpha\beta}(r) = \frac{e^2}{r}\left(1 - \exp\left(-\frac{r}{\lambda_{\alpha\beta}}\right)\right) + \delta_{\alpha\beta}\delta_{e\alpha}\ln(2) k_B T \exp\left(-\frac{r^2}{\pi \ln(2) \lambda_{\mathrm{ee}}^2}\right), \tag{2.2}$$

The effective semi-classical potential was obtained by the following method. A spline interpolation of the potential (2.2) and the expression (2.1) was performed at the intersection point (see, for instance, [4]). Note that the effective semiclassical potential is rapidly decreasing with increasing distance due to screening effects. In fact, due to the consideration of three-particle correlations, the effective potential shows stronger screening than the Debye–Hueckel potential where only two-particle correlations are included.

3. Computer simulation results

The coupled equations of motion for $N = 2000$ (sometimes for $N = 5000$) particles ($N/2$ electrons and $N/2$ protons) in the system were integrated numerically by a standard symmetric and antisymmetric Verlet's algorithm with an integration step of $\Delta t^* = 0.01$—0.05. The time step was chosen from considerations of conservation of the system's total energy. A typical calculation covers several hundred electron plasma oscillations. Periodic boundary conditions were used. Finally, as a result of integration of the equations of motion we have the coordinates $\mathbf{r}_{\mathrm{i}}(t)$ and velocities $\mathbf{v}_{\mathrm{i}}(t)$ dependent on the time for all N particles ($i = 1, 2, \ldots, N$).

The dimensionless values of the electron mean square displacements of the coordinates (in units of a^2) are shown in Fig. 1. Note that mean square displacements increase linearly up to a typical value of time t_{m} which can be interpreted as a dynamical memory time. From this time on, the influence of initial conditions on the dynamical processes in the system can be neglected, i.e. the system 'forgets' its initial state. The system is then in a quasi-equilibrium state, the particles are distributed uniformly on average and the self-diffusion coefficient can be estimated.

In order to investigate dynamic and transport properties we have calculated the velocity autocorrelation functions (VAFs) for the plasma particles. In general, we have to calculate electron and ion VAFs. Due to the great difference between the relaxation times of the plasma components ($\tau_{\mathrm{ee}} \ll \tau_{\mathrm{ii}} \ll \tau_{\mathrm{ei}}$) the convergence of the ion VAFs is slow. Thus in the present work we calculate only the VAF for different initial states. The knowledge of the electron VAF is sufficient for the study of transport coefficients such as self-diffusion and electrical conductivity, because these coefficients are determined mainly by the electron component of the

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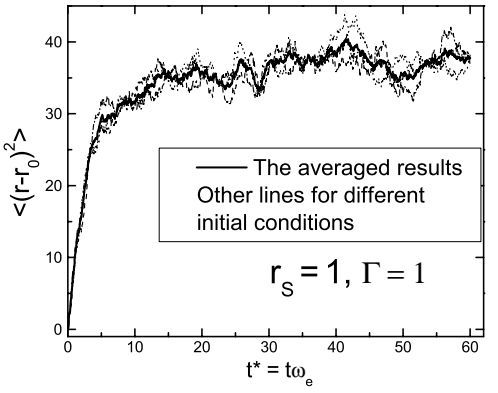

Figure 1. The mean square displacement of coordinates as a function of time.

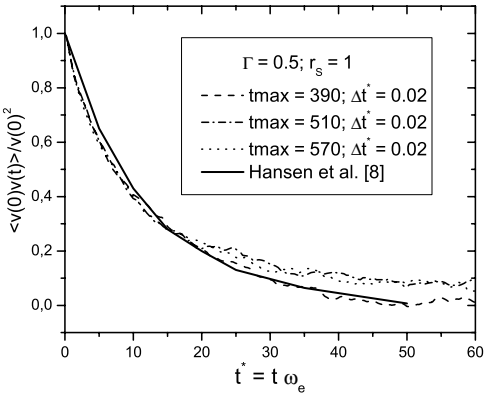

Figure 2. VAF function for different lengths of molecular dynamics runs $t_{\max}$ in units of ω_e.

plasma and the contribution of the heavy ions is negligible. Figures 2 and 3 show the electron VAF for different coupling and density parameters.

We have compared our results with molecular dynamics data of Hansen et al. [8, 9] and reasonable agreement is achieved (see Fig. 2). It is seen that the VAF is monotonic up to $\Gamma \approx 5$. From $\Gamma = 5$ the VAF has a pronounced peak at $t^* \approx 4$ (see Fig. 3). This peak is not connected with the statistical error for the VAF which is obtained as $\sim 1/\sqrt{N} \leqslant 2\%$. We have investigated such a behaviour of the VAF in detail and we found that this peak is independent of the particle number N. This feature can, thus, be interpreted as the onset of collective oscillations in a dense plasma. For a more detailed analysis, it is necessary to investigate the spectral characteristics of the system (e.g. perform a Fourier analysis of the VAF, study the static and dynamic structure factors, etc.). On the basis of the microscopic autocorrelation functions and using the Green–Kubo linear response theory we have calculated the self-diffusion coefficient and the electrical conductivity (Fig. 4) of dense semiclassical plasmas. In Fig. 4 the dimensionless electrical conductivity is presented as function of the coupling parameter. Note that we have good agreement with Spitzer's theory for small values of Γ. We also compare our results with Hansen et al.'s molecular dynamics data based on the semiclassical effective potential and

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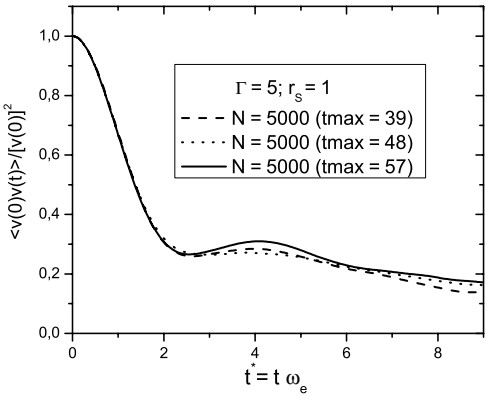

Figure 3. Velocity autocorrelation function for different lengths of molecular dynamics runs t max in units of ω_e.

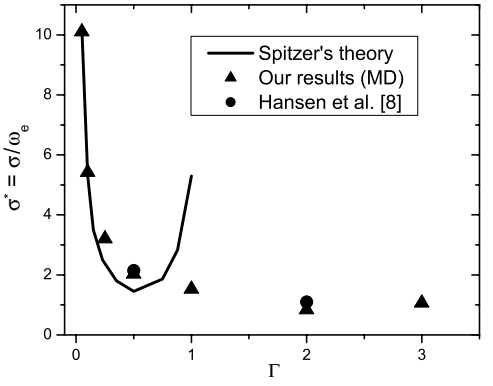

Figure 4. Electrical conductivity of a dense semiclassical hydrogen plasma.

using the standard Ewald summation procedure [8, 9]. At $\Gamma = 0,5$ we have a reasonable agreement but at $\Gamma = 2$ the difference between our and their results is about 20%. It is possible that these deviations are connected with the different interaction models that are used in each work. The results of the present molecular dynamics simulations show that the semiclassical effective potential which takes into account diffraction and symmetry effects at short distances and collective many-particle screening effects at large distances can be adequately used for the description of microscopic and transport properties of a dense, strongly coupled hydrogen plasma.

Finally, we discuss briefly the differences between the pseudopotentials utilized in this work and those used by Hansen et al. [8]. Their pseudopotentials also account for diffraction and symmetry effects but not for screening effects in the plasma, and behave like the Coulomb potential for $r \to \infty$. In this context the Ewald procedure as used in [8] is summing up the long-range interactions. The effective potential that we use in our present work contains quantum diffraction and symmetry effects at short distances as well as many particle screening effects for large distances. Thus, there is no need to use the Ewald method in our case. In this work we have

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revealed no new effects in the behaviour of the electrical conductivity up to $\Gamma \sim 3$. However, at $\Gamma \geqslant 5$ we observe new effects related to oscillations of the VAF (Fig. 3). On should note that this fact can be explained by the formation of quasi-ordered structures and by collective oscillations of the electrons in a dense plasma. We may expect new effects in the behaviour of physical properties (electrical conductivity, diffusion, etc.) for the following parameters of plasma: $\Gamma \geqslant 5$; $r_s = 1{-}5$. This is what we will aim at in our future investigations.

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