Molecular dynamics calculation of the thermal conductivity and shear viscosity of the classical one-component plasma

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The thermal conductivity \( \lambda \) and shear viscosity \( \eta \) of the three-dimensional classical one-component plasma (OCP) were determined by molecular dynamics experiments. In the simulations the velocity of the particles was spatially modulated, and the transport coefficients were calculated from the relaxation time of the modulation profile. The results are given for the \( 2 \leq \Gamma \leq 125 \) range of the plasma coupling parameter \( \Gamma \). The reduced shear viscosity \( \eta^* \) was found to exhibit a minimum at \( \Gamma = 20 \) in agreement with previous calculations. In the \( 2 \leq \Gamma \leq 10 \) range our method yields \( \eta^* \) values 20%–50% higher compared to some of the previously obtained data, while very good agreement was found at the position of the minimum of \( \eta^* \). The reduced thermal conductivity \( \lambda^* \) exhibits a minimum (similarly to \( \eta^* \)) at \( \Gamma \) between 15 and 20. The calculations presented here result in 30%–40% lower thermal conductivity compared to previously available data.

I. INTRODUCTION

One-component plasmas (OCP) consist of a single species of charged particles immersed in a uniform, neutralizing background of oppositely charged particles.\(^1\)\textsuperscript{–}\(^3\) The OCP model can be used to describe different physical systems occurring in nature, e.g., stellar interior,\(^4\) liquid metals\(^5\) electron layers on the surface of liquid helium,\(^6\)\textsuperscript{–}\(^7\) ions stored in traps,\(^8\)\textsuperscript{–}\(^9\) and particles in dusty plasmas.\(^10\)

In the case of pure Coulombic interaction, the properties of the classical OCP are exclusively determined by the dimensionless plasma coupling parameter \( \Gamma \) (expressing the ratio of the potential energy of particles to their kinetic energy). Assuming that the particles are singly charged, \( \Gamma \) is given by

\[
\Gamma = \frac{1}{4 \pi \varepsilon_0} \frac{e^2}{a k_B T},
\]

where \( e \) is the elementary charge, \( \varepsilon_0 \) is the permittivity of free space, \( k_B \) is the Boltzmann constant, \( T \) is the temperature (all units given in SI) and \( a \) is the Wiegner–Seitz (ionsphere) radius,

\[
a = \left( \frac{3}{4 \pi n} \right)^{1/3},
\]

where \( n \) is the number density of the system.

For \( \Gamma \) values below 1 the plasma is said to be weakly coupled, while \( \Gamma \geq 1 \) represents the strong coupling regime where the potential energy of the particles dominates over their kinetic energy.

The total internal energy \( U \) and the pressure \( p \) of the OCP are given by\(^1\)

\[
U = \frac{1}{2} N k_B T + U_{ex},
\]

\[
p = n k_B T + \frac{U_{ex}}{3V},
\]

where \( N \) is the number of particles, \( V \) is the volume, and

\[
U_{ex} = f(\Gamma) N k_B T
\]

is the excess internal energy (resulting from the “potential” interaction of the particles). The \( f(\Gamma) \) function can be approximated for the \( 1 \leq \Gamma \leq 160 \) range by

\[
f(\Gamma) = A \Gamma + B \Gamma^{1/4} + C \Gamma^{-1/4} + D,
\]

where \( A = -0.897 52, B = 0.945 44, C = 0.179 54, \) and \( D = -0.800 49 \)\(^11\)

Simulation techniques, like Monte Carlo\(^12\)\textsuperscript{–}\(^19\) and molecular dynamics\(^20\)\textsuperscript{–}\(^24\) methods have extensively been used to explore the behavior of one-component plasmas. The equation of state and several thermodynamic and transport parameters were obtained from these simulations\(^1\)\textsuperscript{–}\(^3\).

The first calculations for the viscosity and thermal conductivity of the classical OCP were carried out in the 1970s. Vieillefosse and Hansen\(^21\) investigated the transverse and longitudinal current correlation functions of the plasma to obtain the shear (\( \eta \)) and bulk (\( \zeta \)) viscosity. They found that the shear viscosity exhibits a minimum at \( \Gamma = 20 \). The other main finding of their work was that the bulk viscosity is orders of magnitude smaller compared to the shear viscosity. The calculations of \( \eta \) by Wallenborn and Baus\(^25\),\(^26\) were based on the kinetic theory of the OCP. Their results were in a factor of three agreement with the previous results\(^21\) at \( \Gamma = 1 \) and within a factor of 2 agreement at \( \Gamma = 160 \). The minimum value of \( \eta \) agreed well for both reports, however the position of the minimum was reported by Wallenborn and Baus\(^25\) to occur at a lower value, \( \Gamma \approx 8 \).
The first data for the transport coefficients obtained from molecular dynamics simulations (and to our best knowledge the very first results for the thermal conductivity) were that of Bernu, Vieillefosse, and Hansen.27,28 Their results were deduced from Kubo currents in the plasma, and were given for only three values of $\Gamma$: 1, 10, and 100.4. The results confirmed that the bulk viscosity is negligible compared with the shear viscosity and showed that the thermal conductivity ($\lambda$) has a minimum around $\Gamma \sim 10$, similarly to the shear viscosity.

In a recent paper we reported a novel calculation method of the thermal conductivity of the classical OCP.29 In contrast to the molecular dynamics studies of Bernu et al.,27,28 where the transport coefficients were obtained from the simulation of an equilibrium system, we applied a perturbation to the system and deduced $\lambda^*$ from the relaxation time of the system towards the equilibrium state. Here we present results of simulations for an extended range of $\Gamma$ and also report calculations of the shear viscosity ($\eta^*$) of the OCP, based on the same principle.

The method of our simulations is described in Sec. II. The results are presented and discussed in Sec. III. The summary of the work is given in Sec. IV.

II. SIMULATION METHOD

Our molecular dynamics simulations were based on the particle–particle particle–mesh (PPPM) algorithm.30–32 This method makes it possible to simulate large ensembles of particles even in the presence of long-range (e.g., Coulombic or gravitational) interaction potentials. In the PPPM method the force of interaction is not truncated, but it is decomposed to a slowly varying part represented on a mesh (mesh-force) and a properly chosen short range correction force which — together with the mesh force — represents the interaction force for the particle pairs accurately.31,32 In the PPPM algorithm periodic boundary conditions are applied to the simulation box. As the finite Fourier transform (FFT) method is applied for the calculation of the slowly varying part of the force, periodic images of charges are automatically included. Our investigations were carried out with two different system sizes (number of particles), $N=1024$ and $N=8192$. The length of the edge of our simulation box (cube) was $L = 10^{-8}$ m. We used a $16^3$ mesh for $N=1024$ and a $32^3$ mesh for $N=8192$ in the PPPM code to optimize the runtime of the simulations.32 Following the method of Hockney and Eastwood32 the simulation time step ($\Delta t$) was chosen taking into account the plasma frequency of the system, the frequencies associated with the closest approach of pairs of particles, and the vibration of pairs of particles at average separation. In the simulations reported here $\Delta t$ ranged between $1.6 \times 10^{-14}$ s and $5.7 \times 10^{-14}$ s for $N=8192$ and it was between $2.5 \times 10^{-14}$ s and $10^{-13}$ s for $N=1024$.

The simulations were started from a bcc crystal configuration of the particles having initial velocities randomly sampled from a Maxwellian distribution corresponding to the specified value of the initial temperature. The thermalization of the system at the beginning of the simulations was checked by monitoring the pair correlation and the velocity distribution functions of the particles. By the 400th (for $N=8192$) or 1000th time step (for $N=1024$) the system was found to be perfectly thermalized and reached a steady temperature $T_0$. At this time ($t=t_0$) a perturbation was applied to the system. For the thermal conductivity experiments the velocity of the particles was perturbed to obtain a sinusoidal spatial temperature profile $[T(x)]$ in the $x$ direction. For the shear viscosity experiments the $y$ component of the velocity of the particles was changed along the $x$ axis.

The simulation box was divided into 8 slabs along the $X$ axis — as it is shown in Fig. 1 — and in each of these slabs a different temperature was set according to

$$T(x_k) = T_0 + T_{M0} \sin \left( \frac{2 \pi x_k}{L} \right), \quad (7)$$

where $T_{M0}$ is the amplitude of the temperature modulation and $x_k (k=1,2,\ldots,8)$ are the midpoints of the slabs along the $X$ axis. At the time of the perturbation the total kinetic energy of the system was not changed.

Similarly to this, in the case of shear viscosity “experiments”

$$W(x_k) = W_{M0} \sin \left( \frac{2 \pi x_k}{L} \right), \quad (8)$$

was set, where $W = \langle v_{xy} \rangle_{i=1,N}$, $v_{xy}$ being the $y$ velocity component of the $i$th particle, and $W_{M0}$ is the amplitude of
the velocity modulation. Note that the average $y$ velocity $\langle v_y \rangle$ is zero before the modulation. The results reported here were obtained with 25% modulation depth, i.e., $T_{M0}/T_0 = 0.25$ and $W_{M0}/(\langle |v_x| \rangle) = 0.25$.

After the modulation the $T(x,t)$ temperature profile or the $W(x,t)$ velocity profile was measured at each time step, a sinusoidal function was fitted to it, and its harmonic amplitude $T_M(t)$ or $W_M(t)$ was determined. The amplitudes of the modulation profiles $T_M(t)$ and $W_M(t)$ were found to fall exponentially for the experimental conditions discussed here, i.e., to follow the

$$T(x,t) = T_{M0} \sin \left( \frac{2 \pi x}{L} \right) \exp \left( - \frac{t-t_0}{\tau_H} \right),$$

solution of the one-dimensional heat-conductivity equation,

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c} \frac{\partial^2 T}{\partial x^2},$$

and in the case of “viscosity measurement” the

$$W(x,t) = W_{M0} \sin \left( \frac{2 \pi x}{L} \right) \exp \left( - \frac{t-t_0}{\tau_s} \right)$$

solution of the shear viscosity equation,

$$\frac{\partial v_x}{\partial t} = \frac{\eta}{p} \frac{\partial^2 v_x}{\partial x^2},$$

where $c$ is the heat capacity, $\rho$ is the mass density, $\tau_H$ and $\tau_s$ are the characteristic times of the relaxation in the thermal conductivity and shear viscosity experiments, respectively. The transport coefficients can be calculated from the relaxation times as

$$\lambda = \frac{cp}{\tau_H} \left( \frac{L}{2 \pi} \right)^2,$$

and

$$\eta = \frac{\rho}{\tau_s} \left( \frac{L}{2 \pi} \right)^2.$$

In Eq. (10) the heat capacity at constant pressure is usually used. In our experiment, however, together with the temperature both the total internal energy ($U$) and the pressure ($p$) are spatially modulated [see Eqs. (3) and (4)]. On the other hand, we have checked that the number of particles ($N_f$) did not change during the “experiments” in each of the slabs in the simulation box, i.e., the number density of the system can be considered homogenous (neglecting the small spontaneous fluctuations). Thus the use of specific heat at constant volume ($c_v$) is appropriate in Eqs. (10) and (13).

The specific heat $c_v$ of the OCP can be calculated as

$$M c_v = \frac{\langle \partial U / \partial T \rangle_v}{\langle f \rangle_v} = N k_b \left[ \frac{3}{2} + f(\Gamma) - \Gamma \frac{\partial f(\Gamma)}{\partial \Gamma} \right],$$

where $M$ is the mass of the system.

Figure 2 illustrates the simulation method described above for the case of a thermal conductivity experiment. Figure 2(a) shows the $T(x,t)-T_0$ temperature distribution plotted for $\Gamma = 3.9$. Figure 2(b) displays the logarithm of the $T_M(t)$ amplitude of the sinusoidal function fitted to $T(x,t)-T_0$ at each time step. The relaxation time $\tau_H$ was determined by fitting a straight line to $\ln[T_M(t)]$. It can be seen in Fig. 2(b) that $\ln[T_M(t)]$ can be fitted by a straight line for a reasonable time interval. However, as $T_M$ decreases the fluctuations make the fitting more uncertain. Thus the fitting was executed for the time interval $t_0 < t < t_1$, where $t_1$ is defined by $T_M(t_1) = T_M(t_0)/e$ ($e = 2.718$). The 25% modulation depth ensured $T_M(t_0) = 35$ K at the time of modulation ($t_0$) and thus it gave $\sim 10:1$ signal to noise ratio in the measurement of $T_M(t)$ which decreased at $t > t_0$. Similar signal to noise ratio was found for the other values of $\Gamma$ using the 25% modulation depth.

The solutions of the heat-conductivity (10) and shear viscosity (12) equations, respectively, were obtained by assuming that $\lambda$ and $\eta$ are independent of the temperature. The “experimentally” obtained exponential fall of $T_M(t)$ and $W_M(t)$ indicates that this is a reasonable approximation in
the solution of (10) and (12). The assumption of a constant \( \lambda \) and \( \eta \) would be more accurate at lower modulation depth \((T_{M0}/T_0\) and \(W_{M0}/\langle |v_z| \rangle)\), however, we found that the 25\% modulation depth was necessary so ensure that the modulation dominates over the spontaneous fluctuations.

It is noted that for \( N=8192 \) a small positive drift of the system temperature \((T_0)\) was observed in our simulations. This drift was most pronounced at low temperatures, it was 1\%–2\% over the relaxation time \(\tau_H\) (or \(\tau_S\)) at the highest \(\Gamma\) \((\Gamma\approx20\) for \(N=8192\)) and became even less important at higher temperatures. The drift (which possibly originates from the unavoidable numerical errors in the simulations) could not be eliminated using shorter time steps. Using a smaller number of particles the drift decreased significantly and allowed us to study the OCP at the \(25\%\) deep perturbation of the temperature all the parts of the system were still in the fluid state.

### III. RESULTS AND DISCUSSION

In this section the results of our calculations are presented and compared with previous results. We also discuss the limitations of our method.

In the case of \(N=8192\) four simulation runs were carried out for each value of \(\Gamma\) and the results and the error bars presented in the forthcoming figures represent the average and the standard deviation of the data obtained from the simulations. For \(N=1024\) the number of runs was 72, first 9–9 runs were averaged; the results and error bars represent the average and standard deviation of 8 data values obtained this way. The standard deviation of the results \((\sigma)\) ranges between 5\% and 20\% at the different values of \(\Gamma\).

Figure 3(a) shows the relaxation times \(\tau_H\) and \(\tau_S\) obtained from our calculations for both system sizes \((N=1024\) and 8192\). The time units are given as the inverse of the plasma frequency \(\tau_P=\omega_P^{-1}\) in Fig. 3. Our method is expected to yield correct transport coefficients when the relaxation time of the modulation profile \((\tau_H\) or \(\tau_S\)) is much longer than the “local” thermalization time in the system. The speed of the local thermalization can be investigated by calculating the velocity autocorrelation function of the particles. Figure 3(b) shows the velocity autocorrelation function \(A_{\psi}(\tau)=\langle \psi(t)\psi(t_0+\tau)\rangle/\langle \psi(t_0)\rangle^2\) (where \(\langle \rangle\) denotes average over the particles) for different values of \(\Gamma\). The velocity autocorrelation time \(\tau_C\) [defined as \(A_{\psi}(\tau_C)=1/\epsilon;\ \epsilon=2.718\)] is also plotted in Fig. 3(a) as a function of \(\Gamma\). It can be seen in Fig. 3(a) that with increasing \(\Gamma\) the velocity autocorrelation time \(\tau_C\) decreases as the collisions between the particles become more frequent and the information about the initial velocity of the particles is lost on a shorter time scale. At \(\Gamma\approx20\) the autocorrelation time is approximately constant, \(\tau_C/\tau_P\approx2\).

At \(\Gamma\approx1\), in the system of 8192 particles the relaxation time of the temperature profile is \(\tau_H/\tau_P=20.4\), but in the system of 1024 particles it is only \(\tau_H/\tau_P=7.7\). This latter value is comparable to the velocity autocorrelation time \(\tau_C/\tau_P=5.6\). We found that this results in different values for the transport coefficients for different system sizes; in smaller system lower values of \(\lambda\) and \(\eta\) are obtained. With increasing \(\Gamma\) \(\tau_C\) decreases [see Fig. 3(a)] and the simulations give an increasing \(\tau_H\) and \(\tau_S\). This behavior at \(\Gamma\approx2\) already results in an order of magnitude longer relaxation time compared to the velocity autocorrelation time. On the basis of this analysis we accepted the results for which the \(\tau_H/\tau_C\geq10\) or the \(\tau_S/\tau_P\geq10\) condition was fulfilled. The transport coefficients calculated taking into account this condition agreed within error bars for the different system sizes. Our previously calculated values of the thermal conductivity \(29\) in the \(1\leq\Gamma\leq2\) range are however, most likely slightly underestimated.

In the forthcoming figures the thermal conductivity \(\lambda\) and the shear viscosity are given in reduced units,

\[
\lambda^* = \frac{\lambda}{n k_B \omega_P a^2}, \tag{16}
\]

\[
\eta^* = \frac{\eta}{n m \omega_P a^2}, \tag{17}
\]
where $m$ is the mass of the particles and $\omega_p$ is the plasma frequency, $\omega_p^2 = ne^2/\varepsilon_0 m$.

The thermal conductivity of the OCP as a function of $\Gamma$ is shown in Fig. 4. The $\lambda^*$ values obtained by Bernu et al.,$^{27,28}$ are also displayed in Fig. 4. The stated accuracy of the results of Bernu et al. is 15%. Our results are consistent with the values given by these authors,$^{27,28}$ though we obtained 20%–30% lower $\lambda^*$. $\lambda^*$ exhibits a clear minimum in the $\Gamma = 15$–20 range, as it was predicted previously.$^{27,28}$

The results obtained for the reduced shear viscosity are presented in Fig. 5 together with the results of previous calculations. The best agreement is found between the present results and the molecular dynamics results of Bernu et al.$^{27,28}$ Our results suggest that $\eta$ is $\approx 20$%–30% higher than any previously accepted data in the $\Gamma \approx 10$ range. The position of the minimum ($\Gamma \approx 20$) and the value $\eta_{\min}^* = 0.08$ agree very well for all the calculations. At high values of $\Gamma$ our results lie between the values of Vieillefosse and Hansen$^{31}$ and those of Wallenborn and Baus.$^{26}$

**IV. SUMMARY**

We carried out molecular dynamics experiments to determine the thermal conductivity $\lambda^*$ and shear viscosity $\eta^*$ of the three-dimensional classical one-component plasma (OCP). In our simulations the velocity of the particles was spatially modulated, and $\eta^*$ and $\lambda^*$ were calculated from the relaxation time of the modulation profile. Based on the analysis of the velocity autocorrelation time of the particles, we found that our simulation method is valid in the $2 \leq \Gamma \leq 10$ range. If the local thermalization of the particles is at least an order of magnitude faster than the relaxation of the modulation profiles applied to the system. The results presented here cover almost the entire fluid range of the OCP.

The reduced shear viscosity $\eta^*$ was found to exhibit a minimum at $\Gamma \approx 20$ in agreement with previous calculations. In the $2 \leq \Gamma \leq 10$ range our method yields $\eta^*$ values $20$%–40% higher compared to some of the previously obtained data, while very good agreement was found at the position of the minimum of $\eta^*$.

The reduced thermal conductivity $\lambda^*$ exhibits a minimum similarly to $\eta^*$ at $\Gamma \approx 20$. Our calculations resulted in $30$%–40% lower thermal conductivity compared to previously accepted data.

Our simulation method is not applicable below $\Gamma \approx 2$ with the present number of particles in the system. However, using $N \approx 10^5$–$10^6$ particles reliable results could be expected for $\Gamma \leq 1$ values, as well.

Finally it is noted that in principle the method would be applicable to calculate the bulk viscosity of the OCP. This could be done by applying a longitudinal velocity perturbation (an $x$-dependent modulation of the $V_x$ velocity component). However, as the bulk viscosity is orders of magnitude lower than the shear viscosity, numerical difficulties are expected to arise using this method.

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