Transport Coefficients of the Yukawa One-Component Plasma

Gwenaël Salin*
MAPMO-CNRS (UMR 6628), Département de Mathématiques, Université d'Orléans, BP 6759, 45067 Orléans Cedex, France

Jean-Michel Caillol†
LPT-CNRS (UMR 8627), Bâtiment 210, Université Paris Sud, F-91405 Orsay Cedex, France
(Received 28 July 2001; published 28 January 2002)

We present equilibrium molecular-dynamics computations of the thermal conductivity and the two viscosities of the Yukawa one-component plasma. The simulations were performed within periodic boundary conditions, and Ewald sums were implemented for the potentials, the forces, and for all the currents which enter the Kubo formulas. For large values of the screening parameter, our estimates of the shear viscosity and the thermal conductivity are in good agreement with the predictions of the Chapman-Enskog theory.

DOI: 10.1103/PhysRevLett.88.065002 PACS numbers: 52.27.Gr, 52.25.Fi, 52.27.Lw

Recently, many numerical studies of the Yukawa one-component plasma (YOCP)—i.e., a system made of N identical classical point particles of charge q and mass m which are embedded in a uniform neutralizing background of volume V and which interact via Yukawa pair potentials $v(r) = q^2 \exp(-\alpha r)/r$—have been performed in view of applications for a broad variety of systems, including dusty plasmas, inertial confinement fusion dense plasmas, jovian planets, brown and white dwarfs, etc. The excess free energy f as well as all the thermodynamic properties of the YOCP depend only upon two parameters, namely, the coupling parameter $\Gamma = \beta q^2/a$, where $\beta = 1/kT$ is the inverse temperature and a is the ionic radius ($4\pi\rho a^3/3 = 1$, $\rho = N/V$ number density), and the reduced screening parameter $\alpha^* = \alpha a$. In the special case where $\alpha^* = 0$, one recovers the well-known one-component plasma (OCP) [1]. The other limiting case $\alpha^* \to \infty$ is that of a dilute gas for which simple approximate schemes can safely be used. The thermodynamic and structural properties of the YOCP have been thoroughly studied by means of equilibrium molecular dynamics (EMD) simulations within periodic boundary conditions (PBC) [2,3] and by Monte Carlo simulations on the hypersphere [4]. Reliable estimates of the free energy $f(\Gamma, \alpha^*)$ are thus available in a wide range of (Γ, α^*) [2–4].

By contrast, very little is known about the dynamical properties of the model. In view of hydrodynamical simulations, precise estimates of the transport coefficients of the YOCP are clearly wanted. Attempts to compute the shear viscosity η by means of nonequilibrium molecular dynamics (NEMD) simulations were discussed recently in the literature [5]. In this Letter we present equilibrium molecular dynamics (EMD) computations not only of η, but also of the bulk viscosity ξ and the thermal conductivity λ. It turns out that our results for η differ significantly from those of Ref. [5], a puzzling point which will be discussed later.

As it is well known, the three transport coefficients η, ξ, and λ are given by the Kubo formulas [6–8] :

$$\eta = \frac{\beta}{V} \int_0^\infty \langle \sigma_{xy}(t)\sigma_{xy}(0)\rangle \, dt \,, \tag{1a}$$

$$\xi = \frac{\beta}{9V} \sum_{\alpha,\beta} \int_0^\infty \langle \sigma_{\alpha\alpha}(t)\sigma_{\beta\beta}(0)\rangle \, dt \,, \tag{1b}$$

$$\lambda = \frac{1}{3VkT^2} \int_0^\infty \langle \vec{J}_e(t) \cdot \vec{J}_e(0)\rangle \, dt \,. \tag{1c}$$

In Eqs. (1), $\sigma_{\alpha\beta}$ denotes the Fourier transform of one of the Cartesian components of the pressure tensor at $\vec{k} = \vec{0}$, and $\vec{J}_e$ is the $\vec{k} = \vec{0}$ component of the Fourier transform of the energy current.

Our simulations were performed in a cube of side L with PBC conditions, and we took an explicit account of the periodicity of the system by making use of Ewald sums. We have shown elsewhere that the PBC expression of the Yukawa pair potential reads, up to an additional constant, as [9]

$$v_{\mathrm{PBC}}(\vec{r}) = \frac{4\pi q^2}{L^3} \sum_{|\vec{k}| \le k_0} \frac{\exp[-(\vec{k}^2 + \alpha^2)/4\delta^2]}{\vec{k}^2 + \alpha^2} \exp(i\vec{k} \cdot \vec{r}) + q^2 \sum_{\epsilon = \pm 1} \times \frac{\mathrm{erfc}(\delta \| \vec{r} \| + \epsilon\alpha/2\delta) \exp(\epsilon\alpha \| \vec{r} \|)}{2 \| \vec{r} \|} \,, \tag{2}$$

where the sum in the right-hand side (r.h.s.) runs over the vectors $\vec{k}$ of the reciprocal lattice. The parameter δ is chosen in such a way that the contributions to $v_{\mathrm{PBC}}(\vec{r})$ in the direct space reduce to a single term ([i.e., the second term of the r.h.s. of Eq. (2)] and that the cutoff k_0 on the vectors $\vec{k}$ is not too large. The optimal choice, which ensures a relative precision of the order of $\sim 10^{-6}$ on $v_{\mathrm{PBC}}(\vec{r})$ for all the points $\vec{r}$ inside the simulation cell, is $\delta \times L \sim 5.6$ [9].

The Ewald expressions for the pressure tensor $\sigma_{\alpha\beta}$ and the energy current $\vec{J}_e$ can be obtained by generalizing the pioneer work of Bernu and Vieillefosse on the OCP [8]. The details of the derivation will be given elsewhere, and

we just quote here, as an example, the resulting expression for the $\vec{k} = \vec{0}$ Fourier transform of the pressure tensor:

$$\sigma_{\alpha,\beta} = \sigma^K_{\alpha,\beta} + \sigma^d_{\alpha,\beta} + \sigma^f_{\alpha,\beta}\,, \tag{3a}$$

$$\sigma^K_{\alpha,\beta} = m\sum_{i=1}^{N} v_{i,\alpha} v_{i,\beta}\,, \tag{3b}$$

$$\sigma^d_{\alpha,\beta} = -\frac{q^2}{2}\sum_{i\neq j}\frac{r_{ij,\alpha} r_{ij,\beta}}{\| \vec{r}_{ij} \|}\left[\sum_{\epsilon=\pm 1}\frac{d}{dr}\,\frac{\mathrm{erfc}(\delta \| \vec{r} \| + \epsilon\alpha/2\delta)\exp(\epsilon\alpha r)}{2r}\,\Bigg|_{r=\|\vec{r}_{ij}\|}\right], \tag{3c}$$

$$\sigma^f_{\alpha,\beta} = \frac{2\pi q^2}{L^3}\sum_{i\neq j}\sum_{\|\vec{k}\|\leq k_0}\frac{\exp[-(\vec{k}^2 + \alpha^2)/4\delta^2]}{\vec{k}^2 + \alpha^2}\exp(i\vec{k}\cdot\vec{r}_{ij})\left[\delta_{\alpha,\beta} - \left(\frac{1}{2\delta^2} + \frac{2}{\vec{k}^2 + \alpha^2}\right)k_\alpha k_\beta\right]. \tag{3d}$$

In our simulations, we choose as a unit of length the ionic radius a and as a unit of time $\tau = \sqrt{3}\omega_p^{-1}$ with $\omega_p^2 = 4\pi\rho q^2/m$. The calculations were performed in the microcanonical ensemble, and the trajectories of each of the N particles (and all its images) were computed by a time-symmetrical integer algorithm [10]. This algorithm is symplectic and ensures an exact conservation of the total momentum of the system. The time increment Δt was chosen in such a way as to ensure a good conservation of the energy (typically $\Delta t = 10^{-2}\tau$ leads to fluctuations of $\sim 10^{-7}$ on the average energy). In most of our simulations $N = 500$, but smaller and larger systems were also considered in order to study finite size effects on the transport coefficients. Typically 5×10^5 time steps were generated after a careful equilibration of the system. Each run was divided into statistically independent blocks of $\sim 5 \times 10^4$ time steps, i.e., much larger than the correlation time. The reported errors on the autocorrelation functions and the transport coefficients were obtained by a standard block analysis [7]; they correspond to one standard deviation. As an example of the precision which can be obtained for sufficiently long calculations, we display in Fig. 1 the autocorrelation of the energy current at $(\Gamma = 10, \alpha^* = 0.1)$. The integral of the function over the time reaches a well-defined plateau which allows for an accurate determination of the thermal conductivity. The precision on λ and on the other transport coefficients is typically of the order of $\sim 1\%$ for most of the considered cases.

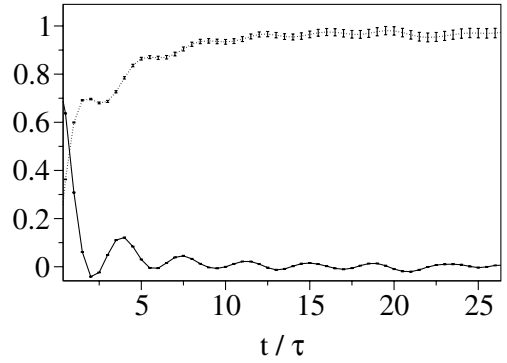

FIG. 1. Solid curve: The autocorrelation function of the energy current $\langle \vec{J}_e(t)\cdot\vec{J}_e(0)\rangle$ for $(\Gamma = 10, \alpha^* = 0.1)$; dotted curve: cumulative sum.

Since the thermodynamic states of the YOCP are characterized by two parameters, a systematic determination of the transport coefficients in the whole fluid phase requires an enormous amount of simulations. We present here only preliminary results for a few thermodynamic states; extended results will be given in a forthcoming publication [11]. Our results are summarized in Tables I, II, and III. We choose the following units: $m\omega_p\rho a^2$ for the viscosities $(\eta = m\omega_p\rho a^2\eta^*,\ \xi = m\omega_p\rho a^2\xi^*)$, $k\omega_p\rho a^2$ for the thermal conductivity $(\lambda = k\omega_p\rho a^2\lambda^*)$.

In order to check our method, we have first considered the case $\alpha^* = 0.01$ and compared our results with those of Bernu and Vieillefosse [8] and of Donkó *et al.* [12] for the OCP. The former authors have performed EMD simulations of the OCP and give estimates of (η, ξ, λ) for a few thermodynamic states, while the latter provide extensive NEMD computations of η and λ. As far as the shear viscosity is concerned, all the results are in overall good agreement except at low Γ's. However, it must be stressed that, in this regime, Bernu and Vieillefosse have considered only relatively small systems of $N = 128$ particles; their results for η are, hence, probably underestimated due to finite size effects. As seen from Table I, the reduced bulk viscosity ξ^* is typically 3 orders of magnitude smaller than η^* which makes difficult its precise determination and entails relatively important statistical errors. Our estimates of ξ^* agree well with those of Bernu *et al.* at large Γ's but, as for the shear viscosity, differ significantly at low Γ's. Finally, our results for the thermal conductivity at $\alpha^* = 0.01$ are in good agreement with those of Bernu *et al.* (except for the lowest Γ's) but are systematically higher than those obtained by Donkó *et al.* in their NEMD simulations [12].

The recent NEMD simulations of Sanbonmatsu and Murillo [5] on the YOCP have been performed only for large values of the screening parameter (i.e., for $\alpha^* = 1, 2, 3,$ and 4. In this case, Ewald sums can probably be safely ignored, at least for sufficiently large systems. Our estimates of the shear viscosity are compared with those of Ref. [5] in Table II for a few thermodynamic states. The disagreement between the two series of simulations is patent, particularly for large values of α^* where the results may differ by a factor of ~ 4. In order to clarify this point, we have focused on the case

TABLE I. Transport coefficients of the YOCP in the limit $\alpha^* \to 0$. The numbers in brackets denote the accuracy of the last digits.

	η			$\xi \times 10^{-3}$		λ		
Γ	YOCP[a]	OCP[b]	OCP[c]	YOCP[a]	OCP[b]	YOCP[a]	OCP[b]	OCP[c]
1	1.16(5)	1.04(21)		4.72(36)	2.6(6)	4.24(29)	2.9(6)	~2.2
2	0.527(7)		~0.5	3.02(5)		1.862(16)		~1.2
10	0.112(1)	0.085(17)	~0.1	1.753(24)	1.8(5)	0.5586(70)	0.66(16)	~0.40
100	0.1874(20)	0.18(3)	~0.18	0.394(7)	0.21(6)	0.843(11)	0.88(17)	~0.72

[a]EMD results at $\alpha^* = 0.01$.
[b]EMD results of Bernu and Vieillefosse [8] for the OCP.
[c]NEMD results of Donkó *et al.* [12] for the OCP.

of the large α^*'s. In this regime, we actually deal with a dilute gas of particles interacting via short range potentials. Clearly, in this case, the transport coefficients can be computed in the framework of the Chapman-Enskog (CE) theory [13]. In the so-called first CE approximation, we have $\xi^* = 0$ and

$$\eta_{\mathrm{CE}} = \frac{5}{8} \frac{kT}{\Omega^{(2)}(2)}, \tag{4}$$

where $\Omega^{(2)}(2)$ is a standard collision integral [13]. Note first that $\xi^* = 0$ which is compatible with the low values of the reported data and the steady decay of ξ^* with respect to α^* for a fixed Γ, as seen from Table II. Moreover, it can be shown that the expression (4) of the CE shear viscosity of the YOCP can be rewritten as

$$\eta_{\mathrm{CE}} = \frac{\alpha^{*2}}{\sqrt{\Gamma}} I(\alpha^* \Gamma), \tag{5}$$

where $I(\alpha^* \Gamma)$ is a triple integral that we have computed numerically by Monte Carlo integration methods. In Fig. 2 we display the EMD and CE shear viscosities as functions of α^* for $\Gamma = 2, 10,$ and 50. The agreement between our EMD results and the predictions of the CE theory is obvious for sufficiently large α^*'s. More precisely, the CE estimates seem to be accurate as soon as the coupling parameter $\Gamma \exp(-\alpha^*) \lesssim 0.35$. The CE theory also enables the computation of the thermal conductivity $\lambda_{\mathrm{CE}} = 5 C_v \eta_{\mathrm{CE}}/2$ and we found, as in the case of the shear viscosity, a perfect agreement between our EMD simulations and the CE theoretical predictions in the domain $\Gamma \exp(-\alpha^*) \lesssim 0.35$.

In summary, our EMD results for the transport coefficients of the YOCP are in good agreement with the available data on the OCP in the limit $\alpha^* \to 0$ and also in good agreement with the predictions of the CE theory for large values of α^*, as it should be, and in severe disagreement with the values reported in Ref. [5].

We think that the standard approach used in this work to compute the transport coefficients—i.e., EMD simulations plus Ewald sums—is efficient and reliable for the two following reasons.

(i) The three transport coefficients η, ξ, and λ can be computed in a single run. By contrast, each transport coefficient requires a separate NEMD simulation.

(ii) Thanks to Ewald sums, the simulations can be undertaken for any value of α^* and they require a small number N of particles. By contrast NEMD simulations seem to require larger system sizes which precludes the use of Ewald sums [5,12].

We have indeed checked that finite size effects on the transport coefficients are small as long as $N \geq 256$. For instance, for the state $(\Gamma = 10, \alpha^* = 1)$, we found for the thermal conductivity $\lambda^* = 0.4138(41)$, $0.5556(54)$.

TABLE II. Transport coefficients of the YOCP for few thermodynamic states. For each coefficient; first column: present EMD results; second column: Chapmann-Enskog prediction ($\xi_{\mathrm{CE}} = 0$ not reported); third column (only for η^*) NEMD estimates of Ref. [5]. The numbers in brackets denote the accuracy of the last digits.

			$\Gamma = 2$			
α		η			λ	$\xi \times 10^{-3}$
1	0.496(12)	0.439(64)	0.2340	2.42(12)	1.65(24)	0.834(48)
2	0.991(24)	0.826(48)	0.2646	2.89(17)	3.09(18)	0.756(14)
3	1.282(36)	1.367(94)	0.4760	5.36(29)	5.13(35)	0.694(12)
4	1.935(36)	2.055(152)	0.5496	7.18(23)	7.71(57)	0.447(5)
			$\Gamma = 10$			
α		η			λ	$\xi \times 10^{-3}$
1	0.112(3)	0.047(5)	0.0526	0.570(18)	0.176(18)	1.282(48)
2	0.145(3)	0.117(10)	0.0521	0.644(17)	0.438(39)	1.205(48)(14)
3	0.198(3)	0.193(10)	0.0693	0.841(18)	0.726(40)	1.426(12)
4	0.306(4)	0.288(19)	0.0870	1.239(23)	1.08(7)	1.255(9)

TABLE III. Transport coefficients of the YOCP for small values of the screening parameter α. The numbers in brackets denote the accuracy of the last digits.

	η			$\xi \times 10^{-3}$			λ		
α	$\Gamma = 2$	$\Gamma = 10$	$\Gamma = 50$	$\Gamma = 2$	$\Gamma = 10$	$\Gamma = 50$	$\Gamma = 2$	$\Gamma = 10$	$\Gamma = 50$
0.2	0.513(5)	0.1054(12)	0.1102(7)	2.78(5)	1.287(24)	0.534(7)	1.716(11)	0.55(1)	0.641(1)
0.4	0.464(5)	0.1033(12)	0.1069(7)	1.439(24)	1.238(24)	0.451(5)	1.96(2)	0.55(1)	0.704(1)
0.6	0.513(5)	0.1093(17)	0.1016(6)	0.967(12)	0.914(17)	0.3906(85)	1.99(2)	0.518(9)	0.560(1)
0.8	0.525(5)	0.1028(15)	0.0937(6)	0.851(5)	0.788(19)	0.372(5)	2.36(2)	0.492(12)	0.592(1)

0.5397(69), 0.5372(56) for $N = 128, 256, 500, 864$, respectively. Therefore systems of $N \sim 500$ are sufficiently large to ensure a reliable estimate of the transport coefficients. Some discrepancies between our results in the case $\alpha^* = 0.01$ and those obtained by Bernu *et al.* for the OCP with systems made of $N = 128$ particles probably originate in finite size effects.

Finally, we have also considered small values of the screening parameter α^*, i.e., $0 \leq \alpha^* \leq 1$. In this case the use of Ewald sums cannot be avoided and some preliminary results are displayed in Table III. Calculations are in progress for other values of (Γ, α^*), and many more results will be given together with a fit of all transport coefficients as functions of (Γ, α^*).

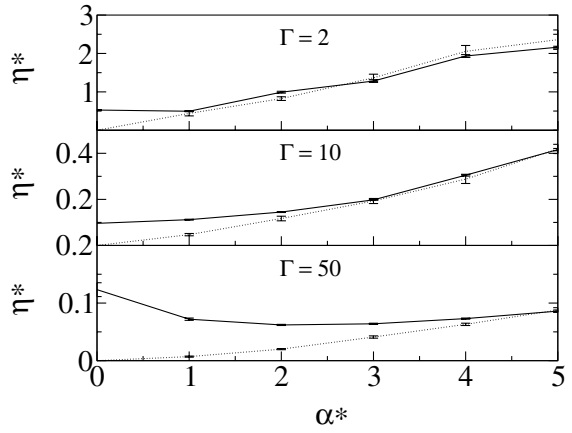

FIG. 2. Shear viscosity of the YOCP as a function of α^* for various Γ's. Solid curve: EMD results; dashed curve: CE theory.

We acknowledge D. Gilles, J. Clérouin, and D. Levesque for useful discussions and D. Levesque for providing us a MD code of the OCP easily transformed in a MD code for the YOCP.

*Email address: salin@labomath.univ-orleans.fr
†Email address: caillol@lyre.th.u-psud.fr

[1] M. Baus and J. P. Hansen, Phys. Rep. **59**, 1 (1980).
[2] S. Hamaguchi and R. T. Farouki, J. Chem. Phys. **101**, 9876 (1994); **101**, 9885 (1994).
[3] S. Hamaguchi, R. T. Farouki, and D. H. E. Dubin, J. Chem. Phys. **105**, 7641 (1996).
[4] J.-M. Caillol and D. Gilles, J. Stat. Phys. **100**, 905 (2000); **100**, 933 (2000).
[5] K. Y. Sanbonmatsu and M. S. Murillo, Phys. Rev. Lett. **86**, 1215 (2001).
[6] J. P. Hansen and I. McDonald, *Theory of Simple Liquids* (Academic, New York, 1986).
[7] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon, Oxford, 1987).
[8] B. Bernu and P. Vieillefosse, Phys. Rev. A **18**, 2345 (1978).
[9] G. Salin and J.-M. Caillol, J. Chem. Phys. **113**, 10 459 (2000).
[10] D. Levesque and L. Verlet, J. Stat. Phys. **72**, 519 (1993).
[11] G. Salin and J.-M. Caillol (to be published).
[12] Z. Donkó, B. Nyíri, L. Szalai, and S. Holló, Phys. Rev. Lett. **81**, 1622 (1998); Z. Donkó and B. Nyíri, Phys. Plasmas **7**, 45 (2000).
[13] S. Chapman and T. Cowling, *The Mathematical Theory of Nonuniform Gases* (Cambridge University Press, New York, 1952).