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Transport coefficients for binary Yukawa mixtures: theory and molecular dynamic simulations

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Abstract

We present the generalization to the binary Yukawa mixture of equilibrium molecular dynamic computations of the transport coefficients of the Yukawa one-component plasma (Salin and Caillol 2002 *Phys. Rev. Lett.* **88** 065002, Salin and Caillol 2000 *J. Chem. Phys.* **113** 10459–63). 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 formulae. Results include shear and bulk viscosities, ionic thermal conductivity, as in the one-component case, but also diffusion and interdiffusion coefficients. We will present the different coefficients and examples of simulations. We shall also compare our simulation results for large screening parameters with Chapman–Enskog theory (Chapman and Cowling 1970 *The Mathematical Theory of Non-Uniform Gases* 3rd edn (Cambridge: Cambridge University Press)).

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1. Introduction

This paper is devoted to the computation of transport coefficients of the model of the binary Yukawa mixture (BYM). This system is made of $N_1 + N_2$ classical point particles of charges q_1 and q_2, and masses m_1 and m_2 which are embedded in a neutralizing background of volume V and which interact via pair potentials

$$v_{ij}(r) = q_i q_j \exp(-\alpha r)/r, \tag{1}$$

where α is the screening parameter. At the thermodynamical limit, the system depends solely on the five following parameters: the screening parameter $\alpha^\star = \alpha a$ (a being the ionic radius), the coupling parameter $\Gamma = \beta e^2/a$ ($\beta = 1/kT$, k is the Boltzmann constant, T is the temperature and e is the electron charge), c the concentration of species 1, $q = q_1/q_2$ and $m = m_1/m_2$, respectively the ratio of charges and the ratio of masses. Note that in the special

case where $\alpha^\star = 0$, one recovers the binary ionic mixture. Another limiting case is when $\alpha^\star \longrightarrow \infty$, where one recovers the case of a dilute gas for which the approximation scheme can be used to compute transport coefficients [3, 4].

Calculation of the transport coefficient for the one-component Yukawa plasma has been made not only theoretically by molecular dynamic simulations [2, 5], but also experimentally by making use of dusty plasma [6, 7]. We here generalize the calculation of the TC of a binary ionic mixture [8] to a binary Yukawa mixture (Yukawa particles), by extending the work done for a Yukawa one-component plasma [2]. Namely, we use equilibrium molecular dynamic (EMD) simulations of a binary Yukawa mixture to compute all the TC. EMD simulations allow us to compute the shear viscosity, the bulk viscosity, the thermal conductivity as in the one-component case, but also diffusion (one component), interdiffusion coefficients and electrical conductivity.

Our simulations are performed within periodic boundary conditions where the trajectories of each particles were computed by the Verlet algorithm [9] and potentials and forces are computed by making use of Ewald sums for the Yukawa potential [1]. As is well known, the transport coefficient (or related coefficients) is given by the Kubo formula [8]

$$\mathcal{TC} = \frac{\beta}{3V}\int_0^\infty \langle J_0(t)J_0\rangle, \tag{2}$$

where $\mathcal{TC}$ is the transport coefficient, V is the volume of a cell, $J_0(t)$ denotes the Fourier transform of the current associated with the $\mathcal{TC}$ at $\mathbf{k} = 0$ and the brackets denote an ensemble average at equilibrium. We also make use of Ewald sums to compute those last currents in our simulations [1].

2. Numerical results

2.1. The transport coefficients of a binary mixture

We define a set of six coefficients: η, ξ the shear and bulk viscosities, and four diffusion coefficients, namely, $l_{11}, l_{1q} = l_{q1}, l_{qq}$ (where the subscript q makes reference to the thermal current and the subscript 1 to one of the species). l_{11} is the diffusion coefficient which is related to the electrical conductivity l_{zz} in the case of charged mixtures. More precisely,

$$l_{zz} = \left(\frac{q_1}{m_1} - \frac{q_2}{m_2}\right)^2 l_{11}. \tag{3}$$

l_{1q} is related to the Soret and Dufour effects (effects taking into account the coupling between the thermal effect and concentration effect). Finally, the thermal conductivity λ can be written in the form

$$\lambda = \frac{1}{T}\left(l_{qq} - \frac{l_{1q}}{l_{11}}\right). \tag{4}$$

2.2. Parameters of the simulations

In our simulations, we choose as the unit of length the ionic radius a and as a unit of time $\tau = 3\omega_p^{-1}$ with $\omega_p^2 = 4\pi\rho q^2/m$. The EMD simulations have been performed with a total number of 500 particles, and 500 000 time steps were generated after a careful equilibration of the system (values are chosen in such a way as to minimize size effect and reliable estimate of the TC (see [2])). The time increment Δt was chosen in such a way as to ensure a good conservation of the energy (typically $\Delta t = 0.01$). Because of the large number of parameters, an extensive calculation of the transport coefficient for all reasonable values of those parameters is not feasible.

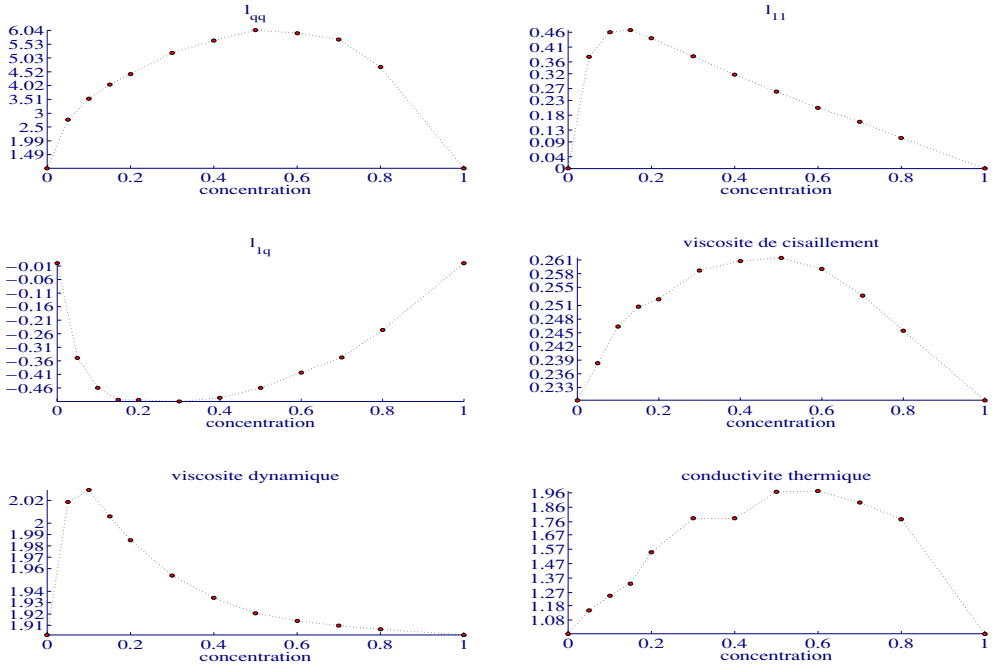

Figure 1. Transport coefficients (from left to right and top to bottom, l_{qq}, l_{11}, l_{1q}, shear viscosity, bulk viscosity, thermal conductivity) as a function of the concentrations c (c in $[0, 1]$), for $\alpha = 1, \Gamma = 5, m = 5, q = 5$.

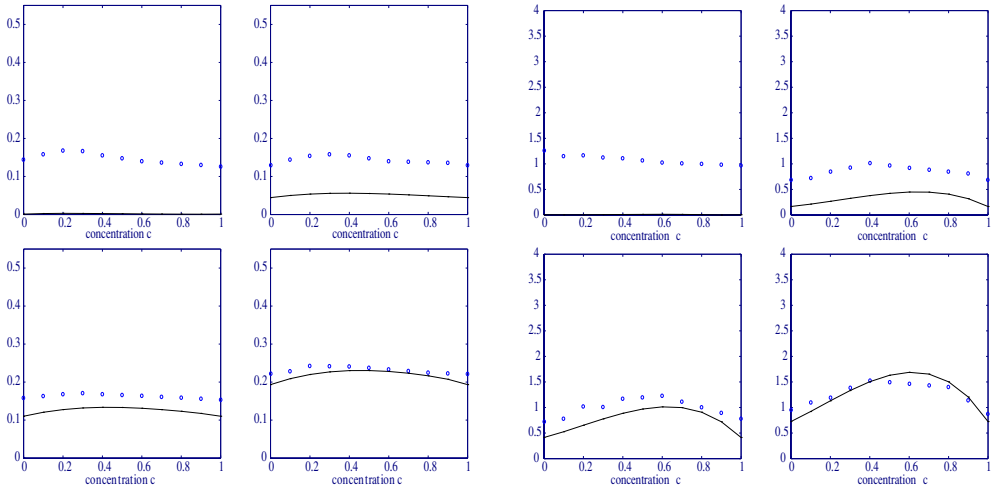

Figure 2. Shear viscosity (four figures on the left) and thermal conductivity (four figures on the right) as functions of the concentration, for several values of $\alpha^\star$ (from left to right and from top to bottom, $\alpha = 0.01, 1, 2, 3$) and for $\Gamma = 10$. Circles EMD simulations, solid curves CE theory.

Then, for preliminary results we choose to fix the ratio of masses m and the ratio of charges q to a representative case of a mixture, namely, $m = 5$ and $q = 5$ (in this particular case the electrical conductivity vanishes (see equation (3))). For those values of ratios, we

perform simulations for the case $\alpha = 1$ and $\Gamma = 5$ and for all concentrations between 0 and 1. Units are chosen so as to recover the limiting case of the YOCP, when c equals 0 or 1. Results for the different coefficients are displayed in figure 1.

2.3. Comparison with CE theory

In the framework of the Chapman–Enskog theory (CET), transport coefficients are expressed as a function of standard collision integrals $\Omega_{ij}^{(l,r)}$ [3, 4]. Then CET provides an approximation scheme for the calculation of the TC. For large values of the screening parameter, we expect that our estimates of the TC are in good agreement with the prediction of the Chapman–Enskog theory. Some tests have been performed in this direction. We have displayed the results found concerning the shear viscosity and the thermal conductivity in figure 2, for $\Gamma = 10$ and $m = q = 5$. As we expected, results are in good agreement when $\alpha \geqslant 2$.

3. Conclusion

We report the first attempt to calculate the full set of common TC of binary Yukawa mixtures by molecular dynamic simulations. The calculations were performed for a mass and charge ratio of 5 and for various concentrations, coupling and screening parameters. These preliminary results of a representative mixture illustrate mass, concentration and screening effects on the TC. Results are in good agreement with earlier calculations of the viscosities and the thermal conductivity [1] and with the limiting case where dilute gas theory can be used. Despite the high time cost of EMD simulations, it stays the most efficient way to compute all the TC.

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