Practical model for the self-diffusion coefficient in Yukawa one-component plasmas

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A practical physically motivated interpolation formula is presented for the self-diffusion coefficient in Yukawa one-component plasmas that is valid for a wide range of inverse screening lengths and over the entire fluid region.

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We report a practical model to estimate the self-diffusion coefficient D in Yukawa one-component plasmas (YOCPs) over a wide range of inverse screening lengths ($0 \leqslant \kappa \leqslant 4$) and across the entire fluid regime. The interpolation formula was obtained by fitting a large body of accurate molecular-dynamics (MD) data. The model was recently discussed in Ref. [1] but was only illustrated for a few values of κ. Here, the four fitting parameters of the model are made into simple functions of κ in order to reproduce the self-diffusion D for any value of κ in the $0 \leqslant \kappa \leqslant 4$ range.

A YOCP consists of an infinite system of classical ions (charge q and mass m) of particle density n at temperature T and in mutual interaction through the Yukawa potential,

$$v(r) = q^2 e^{-\kappa r}/r.$$

The parameter κ mimics the screening effect on the bare Coulomb interactions by the conducting electrons in the plasma; it reduces to either the inverse Debye-Hückel law or the inverse Thomas-Fermi distance in the limiting cases of classical and degenerate electron fluids, respectively. At equilibrium, a YOCP is fully characterized by two dimensionless parameters only, namely, (i) the inverse screening length κ and (ii) the coupling parameter $\Gamma = q^2/ak_BT$, where $a = (4\pi n/3)^{-1/3}$ is the Wigner-Seitz radius. As Γ increases, the Yukawa OCP changes from a nearly collisionless gaseous regime for $\Gamma \ll 1$ through an increasingly correlated liquidlike regime to the crystallization into a lattice at $\Gamma_m(\kappa)$. The values of $\Gamma_m(\kappa)$ considered in the following are those reported in Ref. [2].

To calculate the self-diffusion coefficient, we have performed molecular-dynamics simulations for 10 values of κ in the range of $0 \leqslant \kappa \leqslant 4$ and, for a given κ, for 15 significant values of Γ in the range of $0.1 \leqslant \Gamma \leqslant \Gamma_m(\kappa)$. Our MD simulations are based on a parallel implementation of the particle-particle particle-mesh algorithm that simultaneously treats long- and short-range encounters and allows us to treat both small and large κ values (i.e., long- and short-range interactions) with equal accuracy. The self-diffusion coefficient is obtained using $D = \frac{k_BT}{m}\int_0^\infty Z(t)$, where $Z(t)$ is the normalized velocity autocorrelation function of the species considered. The calculations are performed with enough particles ($5000 \leqslant N \leqslant 200\,000$) over long enough time scales to ensure convergence with a statistical uncertainty of at most $\sim 5\%$ at the smallest couplings ($< 1\%$ elsewhere).

The interpolation formula for $D(\kappa,\Gamma)$ or, more specifically, for the dimensionless quantity $D^* = D/a^2\omega_p$, was obtained by least-squares fitting of the MD data. As discussed in detail in Ref. [1], the model is made of two interpolating formulas that are applicable at small and large couplings, respectively, as follows. In the gaslike small coupling region $\Gamma \leqslant \Gamma^*$, the model extends the popular Chapman-Spitzer (CS) result as follows:

$$D^*(\kappa,\Gamma) = \sqrt{\frac{\pi}{3}}\frac{1}{\alpha(\kappa)}\frac{1}{\Gamma^{5/2}\ln\,\Lambda(\kappa,\Gamma)}, \tag{1}$$

in terms of the generalized Coulomb logarithm,

$$\ln\,\Lambda(\kappa,\Gamma) = \ln\left(1 + C(\kappa)\frac{\lambda_D}{r_L}\right) = \ln\left(1 + \frac{C(\kappa)}{\sqrt{3}\Gamma^{3/2}}\right).$$

As discussed in Ref. [1], the factor α is a correction to the fact that the CS result corresponds to a single Sonine polynomial approximation in the Chapman-Enskog solution of the plasma kinetic equation. The factor C is a correction to the ratio of largest to smallest impact parameters, namely, the Debye length $\lambda_D = \sqrt{4\pi q^2 n/k_BT}$ and the distance of closest approach $r_L = q^2/k_BT$, which are usually introduced somewhat arbitrarily to cut off the divergent collision integrals arising because of the long-range nature of the Coulomb interaction. Here, $\alpha(\kappa)$ and $C(\kappa)$ are fitting parameters,

$$\alpha(\kappa) = \sqrt{\frac{3}{\pi}}\frac{1}{\alpha_0 + \alpha_1\kappa^{\alpha_2}}, \quad C(\kappa) = c_0 + c_1\mathrm{erf}(c_2\kappa^{c_3}),$$

with

$$\alpha_0 = 1.559\,73, \quad \alpha_1 = 1.109\,41, \quad \alpha_2 = 1.369\,09,$$

and

$$c_0 = 2.206\,89, \quad c_1 = 1.351\,594,$$
$$c_2 = 1.571\,38, \quad c_3 = 3.341\,87.$$

As discussed in [1], the effective collision frequency is given by

$$\nu(\kappa,\Gamma)/\nu_0 = \alpha(\kappa)\ln\left(1 + \frac{C(\kappa)}{\sqrt{3}\Gamma^{3/2}}\right),$$

where $\nu_0 = \frac{4}{3}\sqrt{\frac{\pi}{m}}\frac{nq^4}{(k_BT)^{3/2}}$.

In the strongly coupled liquidlike regime, self-diffusion is modeled in terms of thermally activated jumps between equilibrium positions separated by an energy barrier (the so-called cage model) and reads

$$D^* = \frac{A(\kappa)}{\Gamma}e^{-B(\kappa)\Gamma}. \tag{2}$$

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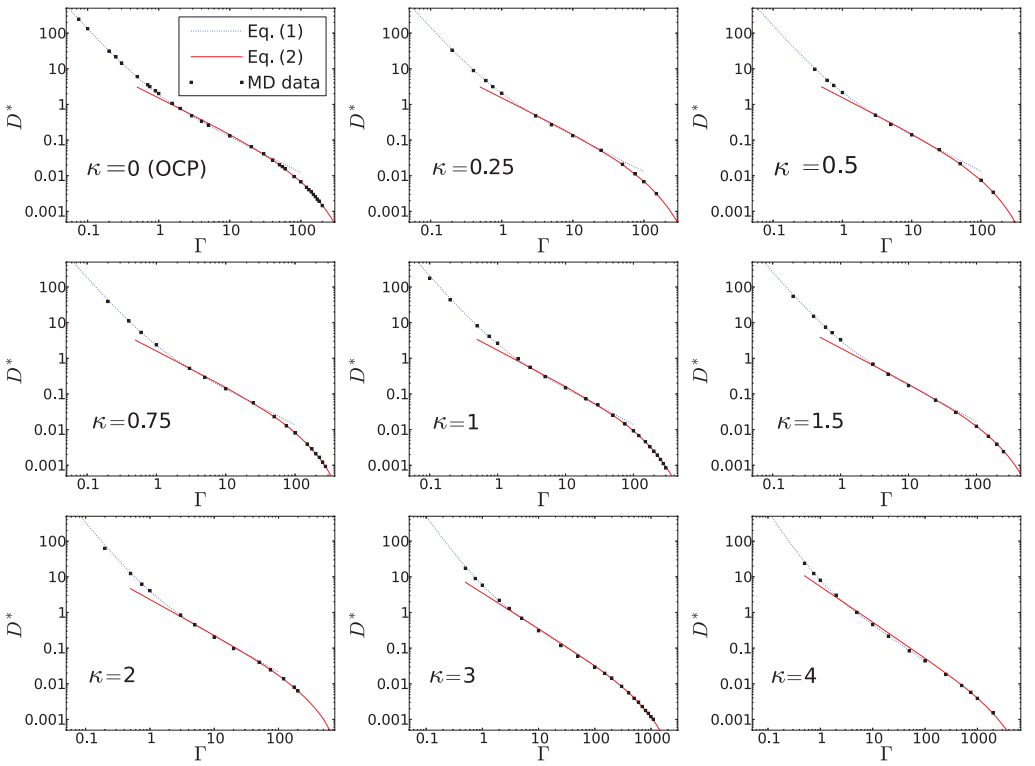

FIG. 1. (Color online) Self-diffusion coefficient $D^* = D/a^2\omega_p$ of the YOCP vs coupling Γ for various κ values as obtained from circles: MD along with the interpolation formulas (1) and (2), respectively, shown by the dashed and solid lines.

As described in Ref. [1], A and B are related to the frequency of jumps from cage to cage [A is related to the transmission coefficient, and B is related to the depth (activation energy) of the cage]. We propose the following parametrization:

$$A(\kappa) = a_0 + a_1\kappa^{a_2}, \quad B(\kappa) = b_0 \exp(-b_1\kappa^{b_2}),$$

with

$$a_0 = 1.525, \quad a_1 = 0.167, \quad a_2 = 2.256\,36,$$

and

$$b_0 = 0.0081, \quad b_1 = 0.292\,124, \quad b_2 = 1.746\,59.$$

Figure 1 shows our MD results for the self-diffusion coefficient D with $0.075 \leqslant \Gamma \leqslant \Gamma_m$ along with the model described.

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