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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 coeffcient 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 estinate the self-diffusion coefficient D in Yukawa one-component plasmas (YOCP) over a wide range of inverse screening lengths ($0 \leq \kappa \leq 4$) and across the entire fluid regime. The interpolation formula was obtained by fitting a large body of accurate molecular-dynamics data. The model was recently discussed in [1] but illustrated for a few values of κ only. 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 $0 \leq \kappa \leq 4$ range.

A YOCP consists of an infinite system of classical ions (charge q, 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 fluid respectively. At equilibrium, a YOCP is fully characterised 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, liquid-like 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 [2].

To calculate the self-diffusion coefficient, we have performed molecular-dynamics simulations for 10 values of κ in the range $0 \leq \kappa \leq 4$ and, for a given κ, for 15 significant values of Γ in the range $0.1 \leq \Gamma \leq \Gamma_m(\kappa)$. 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 (VAF) of the species considered. The calculations are done with enough particles ($5000 \leq N \leq 200000$), 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-square fitting of the MD data. As discussed in detail in [1], the model is made of two interpolating formulas that are applicable at small and large couplings,respectively, as follows. In the gas-like, small coupling region $\Gamma \leq \Gamma^*$, the model extends the popular Chapman-Spitzer (CS) result as follows,

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

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 [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 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,

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

with

$$\begin{aligned} \alpha_0 &= 1.55973 \\ \alpha_1 &= 1.10941 \\ \alpha_2 &= 1.36909 \end{aligned}$$

and

$$\begin{aligned} c_0 &= 2.20689 \\ c_1 &= 1.351594 \\ c_2 &= 1.57138 \\ c_3 &= 3.34187\,. \end{aligned}$$

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Note, as discussed in [1], in this weakly to moderately coupled regime, an 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, liquid-like 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,

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

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

$$A(\kappa) \;=\; a_0 + a_1\kappa^{a_2}$$

$$B(\kappa) \;=\; b_0\exp\left(-b_1\kappa^{b_2}\right)$$

with

$$\begin{aligned} a_0 &= 1.525 \\ a_1 &= 0.167 \\ a_2 &= 2.25636 \end{aligned}$$

and

$$\begin{aligned} b_0 &= 0.0081 \\ b_1 &= 0.292124 \\ b_2 &= 1.74659\,. \end{aligned}$$

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

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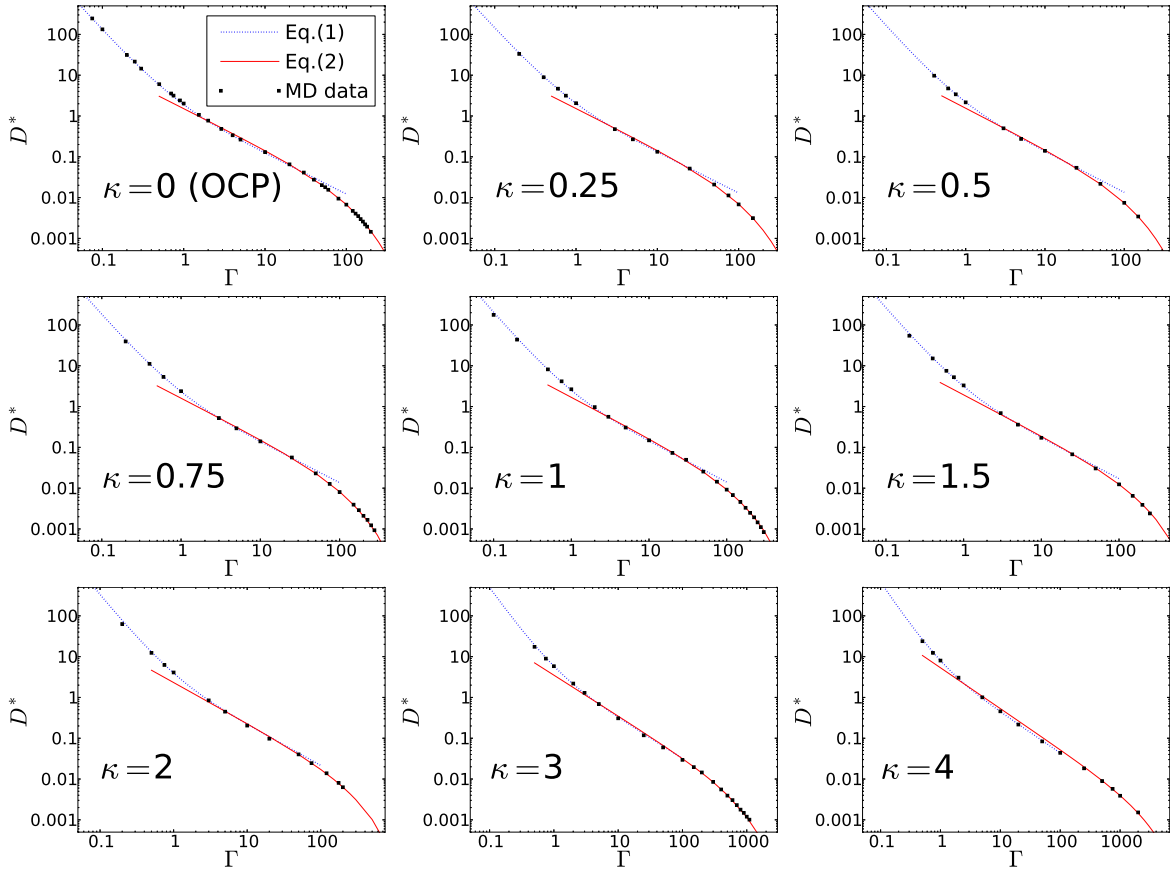

FIG. 1: (color online) Self-diffusion coefficient $D^* = D/a^2\omega_p$ of YOCP vs coupling Γ for various κ-values as obtained from MD (circles), along with the interpolation formulas (1) and (2), respectively shown by the dashed and solid lines.