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LETTER TO THE EDITOR

Quasi-universal melting-temperature scaling of transport coefficients in Yukawa systems

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Abstract

New quasi-universal melting-temperature scalings for transport coefficients in Yukawa systems are presented which test well, and up to $T/T_M \gtrsim 100$, against the recently obtained large body of accurate computer simulation data on self-diffusion and shear viscosity.

Many quite disparate systems of charged particles which are screened by a lighter species can be described by Yukawa interparticle potentials:

$$\frac{\varphi(r)}{k_B T} = \frac{\Gamma}{(r/a_{WS})} \mathrm{e}^{-\alpha(r/a_{WS})}$$

where $\Gamma = Q^2/(a_{WS}k_BT)$ is the coupling strength defined in terms of the charge Q, temperature T, and Wigner–Seitz radius $a_{WS} = (3/[4\pi\rho])^{1/3}$, and α is the screening parameter [1–4]. The classical Coulomb one-component plasma (OCP) corresponds to a Yukawa potential with zero screening, $\alpha = 0$. Systems with repulsive Yukawa potentials make important reference systems in condensed matter physics and provide models for, e.g., dense stellar materials, inertially confined plasmas, 'mesoscopic plasmas' of charge-stabilized colloidal suspensions, and the dusty plasmas of materials processing [5, 6]. In view of their importance within the rapidly evolving field of dusty plasma physics [7] and their relevance for the design of inertial confinement fusion targets [8], there is much interest in the dynamic properties of Yukawa systems, and many computer simulation results for transport coefficients have been obtained very recently by several authors [9–13]. Particularly accurate results were obtained for self-diffusion [11, 12] and shear viscosity [13]. These were found to obey a quasi-universal scaling [14–19], in which reduced (dimensionless) transport coefficients, when plotted as a function of the excess entropy, are only weakly dependent on the interaction potential. The melting-temperature scaling for transport coefficients was recently derived [20] from the excess-entropy scaling, and applied to the new self-diffusion data [12] for Yukawa systems.

Proceeding on from the pioneering work of Hansen and collaborators [21–23], transport coefficients for the OCP and Yukawa systems have been presented (e.g. see references [9–13]) in reduced form involving the plasma frequency, $\omega_p = (4\pi\rho Q^2/m)^{1/2}$, and the Wigner–Seitz radius, a_{WS}. Using the coefficients of thermal conductivity, λ, viscosity, η, and diffusion, D, one defines the following reduced (dimensionless) quantities:

$$\lambda^+ = \frac{\lambda}{\rho k_B \omega_p a_{WS}^2} \qquad \eta^+ = \frac{\eta}{\rho m \omega_p a_{WS}^2} \qquad D^+ = \frac{D}{\omega_p a_{WS}^2}.$$

In this letter I introduce a new (and only slightly modified) set of reduced transport coefficients defined by $t^\# = \Gamma_M^{1/2} t^+$ (where $t = \lambda$, η, or D, and Γ_M is the value of Γ at melting), which provides an insightful tool for analysing the simulation results. Using the recently obtained simulation data for Yukawa self-diffusion [11, 12] and shear viscosity [13] coefficients, I find that $D^\#$ (for $0 \leqslant \alpha \leqslant 5$) and $\eta^\#$ (for $1 \leqslant \alpha \leqslant 4$) as functions of T/T_M (or Γ/Γ_M) are only weakly dependent on the screening parameter α all the way up to $T/T_M \gtrsim 100$ (i.e. $0.01 \lesssim \Gamma/\Gamma_M$).

In view of the absence of a unifying quantitative description of atomic transport in condensed matter [16, 17, 24, 25], the approximate scalings [14] which relate reduced (dimensionless) transport coefficients to the reduced excess (i.e. configurational, over ideal-gas value) entropy, $S^E/(Nk_B)$, enable one to estimate unknown transport coefficients and may provide guidelines for theoretical analysis. *Macroscopic* reduction parameters (density and temperature) were chosen [14]—namely, a mean interparticle distance, $d = (V/N)^{1/3} = \rho^{-1/3}$, and the thermal velocity, $v_{th} = (k_B T/m)^{1/2}$, to define the following reduced transport coefficients:

$$\lambda^* = \lambda \frac{\rho^{-2/3}}{k_B (k_B T/m)^{1/2}} \qquad \eta^* = \eta \frac{\rho^{-2/3}}{(m k_B T)^{1/2}} \qquad D^* = D \frac{\rho^{1/3}}{(k_B T/m)^{1/2}}.$$

These forms of the reduced transport coefficients are suggested by an elementary kinetic theory for a dense medium of particles with thermal velocities but with a mean free path between collisions which is of the order of the average interparticle distance. The excess-entropy dependence of these reduced coefficients was originally suggested [14] by the hard-spheres model, but can also be obtained from cell theory arguments [15–17]. The simulation results for many systems with quite disparate pair interactions show quasi-universal behaviour of the following type [14–19]: let t^* be a reduced transport coefficient ($t = \lambda$, η, or D) as defined above, and $s = -S^E/(Nk_B) \gtrsim 0$; then,

$$t^* \simeq g_t^*(s) \tag{1}$$

where the corresponding function g_t^* is weakly dependent on the potential for all *strongly coupled* simple fluids, i.e. in the range $1 \lesssim s \lesssim s_{freez}$ (freezing corresponds to about $4 \lesssim s_{freez} \lesssim 5$). The recent results for the Yukawa potentials [11–13] also support [13,20] this 'rule' with, moreover, the quasi-universality extending to values of s well below unity. This is not totally unexpected given that the excess-entropy scaling can be shown analytically to be valid also for soft inverse-power potentials in the weak-coupling (dilute-gas) regime [19].

Using density functional theory it was recently predicted [26] that the excess entropy for soft inverse-power potentials and for the Yukawa systems has an asymptotic strong-coupling expansion dominated by a $\Gamma^{2/5}$ (i.e. $T^{-2/5}$) term near freezing. Moreover, it was subsequently found [20] that the simulation data for these systems obey a quasi-universal scaling law of the form

$$s \simeq f(T/T_M) \tag{2}$$

where the function $f \approx s_{freez} + (9/2)[(T/T_M)^{-2/5} - 1]$ is about the same for all relatively soft Yukawa and inverse-power potentials, all the way up to $T/T_M \approx 10$ (i.e. down to $\Gamma/\Gamma_M \approx 0.1$), corresponding roughly to $s \approx 1$. By combining the two *approximate* scaling relations, equation (1) and equation (2), a new *approximate* scaling relation is obtained of the type

$$t^* \simeq G_t^*(T/T_M) \equiv g_t^*(f(T/T_M)) \tag{3}$$

where t^* is a reduced transport coefficient ($t = \lambda$, η, or D) as defined above, and the corresponding function G_t^* is weakly dependent on the potential. This set of reduced transport coefficients is related to the one defined above by the relation

$$t^+ = \frac{(4\pi/3)^{1/3}}{\sqrt{3}\Gamma^{1/2}} t^*$$

where $t = \lambda$, η, or D. If we multiply these by $\Gamma_M^{1/2}$ and define the new set of reduced transport coefficients

$$t^\# = \Gamma_M^{1/2} t^+ = \frac{(4\pi/3)^{1/3}}{\sqrt{3}(\Gamma/\Gamma_M)^{1/2}} t^*$$

we expect quasi-universal relations of the type

$$t^\# \simeq G_t^\#(T/T_M) \equiv \frac{(4\pi/3)^{1/3}}{\sqrt{3}} (T/T_M)^{1/2} G_t^*(T/T_M) \tag{4}$$

up to $T/T_M \lesssim 10$, where $G_t^\#$ is weakly dependent on the Yukawa screening parameter.

It should be emphasized that since each involves two *approximate* scaling relations, the degree of universality of the resulting functions $G_t^\#$ is some combination of the degrees of universality of the functions g_t^* and f, and (as happens for Yukawa systems) may improve upon that of g_t^*. On the basis of its derivation, the range of T/T_M over which the functions $G_t^\#$ will be quasi-universal for the Yukawa systems is expected to be $T/T_M \lesssim 10$. Note also that within the expected degree of universality of the excess-entropy scaling for the Yukawa potentials, similar scaling relations can be obtained by interchanging T_M and the freezing temperatures, T_{freez}.

Using the recent simulation results for the Yukawa transport coefficients [11–13], and the melting temperatures given in [6], the results for the newly defined coefficients $t^\#$ are presented in figures 1 and 2. The quasi-universalities of both $D^\#$ (for $0 \leqslant \alpha \leqslant 5$) and $\eta^\#$ (for $1 \leqslant \alpha \leqslant 4$) hold well for $0.01 \lesssim \Gamma/\Gamma_M$ (i.e. $T/T_M \lesssim 100$). The degree of universality (i.e. the spread of the results for different values of α) is better than for previous scalings [12–14, 20], and holds for temperatures much higher than expected on the basis of its derivation. This rather surprising important property of the Yukawa systems enables one to represent the Yukawa transport coefficients by simple 'wide-range' fitting formulae. Defining $x = \log_{10}(\Gamma/\Gamma_M)$, the full lines shown in the figures represent the following fits:

(1) In figure 1, $\log_{10}(D^\#) = -1.442\,52 - 1.454\,44\,x - 0.097\,31\,x^2$.
(2) In figure 2, $\log_{10}(\eta^\#) = 0.186\,29 + 1.252\,95\,x + 0.876\,59\,x^2 + 0.076\,05\,x^3 - 0.014\,62\,x^4$.

These are only tentative, pending further improvements in the accuracy of the simulation results. For the shear viscosity, in particular, the overall quasi-universality of the data is affected by finite-size effects [13]. All of the results for $\alpha = 1$ in figure 2 are for $N = 25\,600$, which is closest to the hydrodynamic result, while most of the $N = 3200$ results are expected to move slightly higher, by perhaps 20%. It is generally expected [13] that the Yukawa viscosity results are tighter than might be inferred from figure 2 because of the finite length scales used in the simulations. The melting-temperature scaling highlights the discrepancy (as discussed in [13]) between the new and more accurate shear viscosity results for the Yukawa potential [13] and the earlier results for the OCP [9, 10] (in figure 2 they are about a factor of 2.4 above the fitting curve).

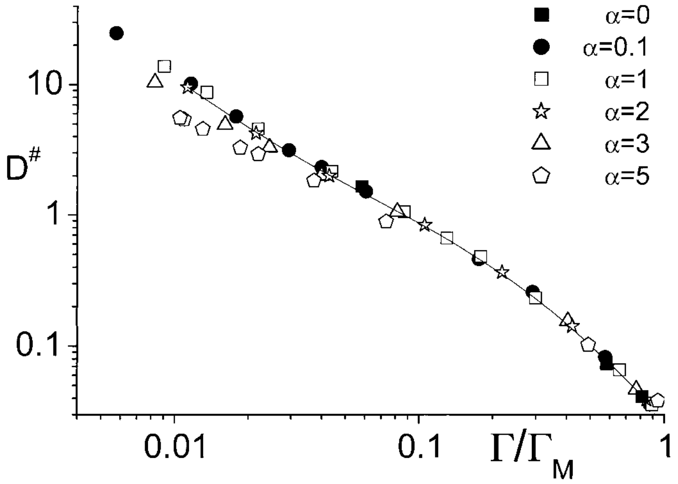

Figure 1. Simulation results [11, 12] for the Yukawa reduced diffusion coefficient $D^{\#}$ as a function of $\Gamma/\Gamma_M = (T/T_M)^{-1}$ for various values of the screening parameter $\alpha > 0$. Also shown are earlier results [18, 21] for the OCP $\alpha = 0$ case. The full line represents a fit. See the text.

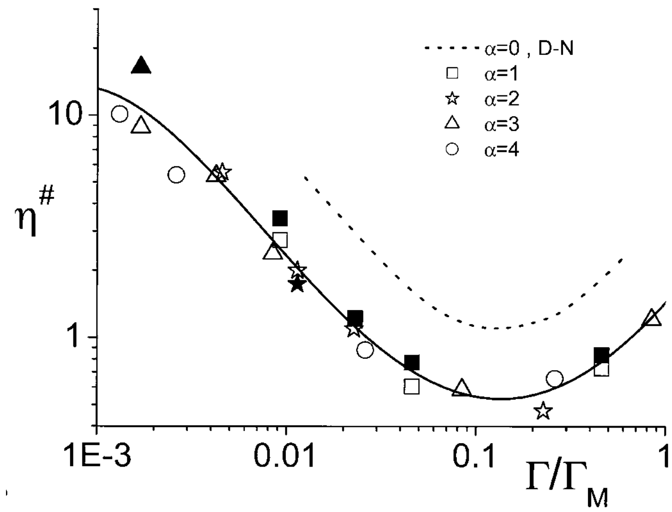

Figure 2. Simulation results [13] for the Yukawa reduced viscosity $\eta^{\#}$ as a function of $\Gamma/\Gamma_M = (T/T_M)^{-1}$ for various values of the screening parameter $\alpha > 0$. The open symbols represent $N = 3200$ data points, while the corresponding filled symbols represent $N = 25\,600$ results. The full line represents a fit. The dotted line represents somewhat earlier results [9, 10] for the OCP $\alpha = 0$ case. The discrepancy between these two sets of data is discussed in [13]. See the text.

It should be noted that the excess-entropy scaling (which leads to the present melting-temperature scaling) *predicts* [19] a quasi-universal minimum in the viscosity for a temperature in the vicinity of $T/T_M \approx 0.1$, as indeed found in figure 2. The same excess-entropy scaling analysis [19] *predicts* also a quasi-universal minimum in the thermal conductivity for $T/T_M \approx 0.1$, which is in general agreement with the $\alpha = 0$ results in [9, 10]. When accurate results for different values of α become available, it will be possible to check the predicted quasi-universal behaviour of the Yukawa thermal conductivity.

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