Stokes−Einstein Relation in Two- and Three-Dimensional Fluids[†]

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The Stokes−Einstein relation, relating the self-diffusion coefficient D to the shear viscosity η ($D = k_BT/2\pi\eta\sigma$), is tested for two- and three-dimensional fluids. The influence of attractive potential and temperature on the validity of the Stokes−Einstein relation by employing square-well potential is analyzed. A breakdown of the Stokes−Einstein relation is observed at low temperatures for three-dimensional fluid by using the Nigra and Evans[11] model and with that obtained from the velocity autocorrelation function[10] and for two-dimensional fluids by using the Garcia−Rojo et al.[12] model for hard discs.

Introduction

The problem of accurately predicting transport properties of simple fluid over a wide range of densities and temperatures has been a central concern in recent years. The transport properties are less amenable to accurate theoretical calculation and require computationally intense molecular dynamic simulations, hence the continuing interest in their study. Through a natural, although adhoc, extension of the dilute gas Boltzmann equation, Enskog transport theory[1] provided the first prediction of the transport coefficients of the hard sphere fluid and opened the way to the calculation of transport properties of real dense fluids. In addition to the aforementioned problems, the transport coefficients tend to make their molecular understanding appear even more complex and discouraging. Therefore, the complex and difficult task would be made less daunting if there were some rigorous or sufficiently accurate relations between the various transport coefficients. One such typical relation is the Stokes−Einstein relation that relates the self-diffusion coefficient D to the shear viscosity η for dense fluid.

The Stokes−Einstein relation for three-dimensional fluids

$$D = \frac{k_BT}{C\pi\eta\sigma} \tag{1}$$

is an important hydrodynamic law relating the diffusion coefficient D of the Brownian particles and the fluid shear viscosity η. This combines the Einstein relation $D = \{k_BT/\xi\}$ for D and Stokes law $\xi = c\eta\sigma$ for the frictional force ξ on a sphere in a fluid. In eq 1, k_B is Boltzmann constant; T is absolute temperature; C is a numerical constant determined by the hydrodynamic boundary condition; and σ is the diameter of the hard sphere particle. In the recent past, the Stokes−Einstein (S−E) relation was supposed to be valid. Now, it has been observed that the S−E relation fails under certain conditions. In the present work, we consider the validity of the S−E relation in the presence of attractive intermolecular forces in a simple derivation of the Stokes−Einstein relation. We consider the square-well fluid in which the time correlation (tcf) of intermolecular forces arises from repulsion and attraction.

Recently, Liu et al. [2] have tested the Stokes−Einstein relation for a 2D Yukawa fluid. In the present work, we have tested the validity of the Stokes−Einstein relation over a wide range of densities for hard discs.

Theory

Knowledge of the velocity time correlation function (tcf) allows calculation of transport coefficients which describe the displacement of mass, momentum, and energy through the system in response to a perturbation. Although the Green-Kubo relations[3,4] are often used to relate the integral of a corresponding time correlation function to its transport coefficient, it is difficult to implement in a reference system such as the hard spheres due to a singularity in the time correlation function. Thus, alternative approaches are considered such as the memory function $R(t)$ is considered rather than the velocity autocorrelation function. Alder et al.[5] used a mean-square displacement approach to calculate transport coefficients of the hard sphere system. Evans[6] employed a generalized Langevin equation of the form[7,8]

$$\frac{d}{dt}C_V(t) = -f_EC_V(t) + \int_0^t d\tau R(t-\tau)C_V(\tau) \tag{2}$$

where $C_V(t)$ is the velocity tcf

$$C_V(t) = \frac{m}{k_BT} < v \cdot v(t)> \tag{3}$$

and m is the mass of the particle; k_BT is the thermal energy; f_E is the Enskog friction drag arising from the uncorrelated binary collisions; and $R(t)$ is the memory function arising from correlated events. The Enskog friction f_E is given by

$$f_E = \frac{2}{3}\pi\sigma^2g^{HS}(\sigma)v_F = \frac{2}{3}Z = \frac{16}{\sqrt{\pi}}yg^{HS}(\sigma)\omega$$

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$$v_F = \sqrt{\frac{16k_B\mathrm{T}}{\pi m}} \text{ and } \omega = \sqrt{\frac{k_BT}{m\sigma^2}} \qquad (4)$$

where Z is the collision frequency per particle; v_F is the relative thermal velocity; $y = (\pi/6)\rho\sigma^3$ is the packing fraction; the contact pair correlation function, $g^{HS}(\sigma)$, for a hard sphere fluid and can be calculated from the Carnahan and Starling equation as

$$g^{HS}(\sigma) = \frac{1 - 0.5y}{(1 - y)^3} \qquad (5)$$

The dynamical variable in the memory function arises from the binary collision operator and is $\check{r}\ \delta(r - \sigma)$, where r is the center-to-center distance for a specific pair of hard spheres and σ is the hard sphere diameter. The decay of the memory function is governed by a time correlation function of the form

$$C_1(t) = <\delta(r - \sigma)P_1(\check{r}\bullet\check{r}(t))\delta(r(t) - \sigma)> \qquad (6)$$

So that the frequency-dependent memory function is

$$\hat{R}(s) = \int_0^\infty \mathrm{d}t \exp(-st)R(t) = -\Omega^2\hat{C}_1(s) \qquad (6a)$$

The $t = 0$ value of the $C_1(t)$ tcf is not trivial to derive. Merely substituting $t = 0$ into the tcf yields infinity. However, the memory function from its zero time value is derived by Tang et al.[9] as

$$R(t = 0^+) = -\Omega^2,\ \Omega = (1/4)f_E \qquad (7)$$

evaluated under the assumption that three-body dynamical events were significant. Using the zero time value of the memory function (eq 6a and 7)

$$\hat{C}_1(s) = \frac{1}{\omega}\hat{h}_1(s) \qquad (7a)$$

Thus, the velocity correlation function can be written as[6]

$$C_V(s) = \left\{s + f_E + \frac{\Omega^2\hat{h}_1(s)}{\omega}\right\}^{-1} \qquad (8)$$

where

$$\hat{h}_1(s) = \frac{1}{1 + x + (1 + x)^{-1}}$$
$$x = \sqrt{\frac{s^2\sigma^2}{2D(s)}}$$

where $D(s)$ is the frequency-dependent diffusion coefficient. Now, the diffusion coefficient can be defined as

$$D = \frac{k_BT}{m}\hat{C}_V(s = 0) \qquad (9)$$

$$\hat{C}_V(s = 0) = \left(0 + \frac{16}{\sqrt{\pi}}yg^{HS}(\sigma)\omega + \frac{16}{\pi}y^2[g^{HS}(\sigma)]^2\omega\hat{h}_1(s = 0)\right)^{-1} \qquad (10)$$

Hence the diffusion coefficient can be solved as

$$D = \left(\frac{k_BT}{m\sigma^2}\right)^{1/2}\sigma^2\left\{\frac{16yg^{HS}(\sigma)}{\sqrt{\pi}} + \frac{8y^2[g^{HS}(\sigma)]^2}{\pi}\right\}^{-1} \qquad (11)$$

and the final expression for the reduced diffusion coefficient can be written as

$$D^{HS^*} = \frac{D}{\left(\frac{k_BT}{m\sigma^2}\right)^{1/2}\sigma^2} = \left\{\frac{16yg^{HS}(\sigma)}{\sqrt{\pi}} + \frac{8y^2[g^{HS}(\sigma)]^2}{\pi}\right\}^{-1} \qquad (12)$$

Here $g^{HS}(\sigma)$ is the pair correlation function for the hard sphere system. We have obtained the self-diffusion coefficient for a square well fluid by using the Chapman−Enskog method of solution by replacing the pair correlation function $g^{HS}(\sigma)$ in eq 12 by $g^{SQ}(\sigma)$ as

$$g^{SQ}(\sigma) = g^{SW}(\sigma) + \lambda^2g^{SW}(\lambda\sigma)E \qquad (13)$$

where $g^{SW}(\sigma)$ and $g^{SW}(\lambda\sigma)$ are the radial distribution functions evaluated at the points σ and $\lambda\sigma$, respectively.

Hence, velocity correlation function for square-well fluids can be written as

$$\hat{C}_V(s = 0) = \left(\frac{16}{\sqrt{\pi}}yg^{SQ}(\sigma)\omega + \frac{16}{\pi}y^2[g^{SQ}(\sigma)]^2\omega\hat{h}_1(s = 0)\right)^{-1} \qquad (14)$$

The reduced diffusion coefficient for square-well fluids can be written as

$$D^{SW*} = \left\{\frac{16yg^{SQ}(\sigma)}{\sqrt{\pi}} + \frac{8y^2[g^{SQ}(\sigma)]^2}{\pi}\right\}^{-1} \qquad (15)$$

For square-well fluid, the pair correlation function $g^{SW}(\sigma)$ can be written in high-temperature approximation (HTA)

$$g^{SW}(\sigma) = g^{HS}(\sigma) + \frac{1}{4T^*}\frac{\partial a_1^{SW}}{\partial\eta} + \frac{\lambda^3}{T^*}g^{HS}(\lambda\sigma) \qquad (16)$$

where a_1^{SW} is the first-order perturbation term associated with attractive energy as given below

$$a_1^{SW} = -4\eta(\lambda^3 - 1)\left\{\frac{1 - 0.5\eta_{\mathrm{eff}}}{(1\text{-}\eta_{\mathrm{eff}})^3}\right\} \qquad (17)$$

where η_{eff} and $g^{HS}(\lambda\sigma)$ are defined in our recent work.[10] Equation 16 is very useful for Chemical Engineers for the chemical products whose theoretical thermodynamic and transport properties do not match with experimental results for square-well fluids.

To calculate the Stokes−Einstein relation values, we have employed the following equation proposed by Evans[6]

$$\frac{2\pi D^{\mathrm{SW}}[\eta^{\mathrm{SW}} - \eta_{\mathrm{E}}]\sigma}{k_{\mathrm{B}}T} = \frac{4yf_{\mathrm{E}}}{25\omega(1 + S)} \tag{18}$$

or

$$\frac{2\pi D^{\mathrm{SW}}\eta^{\mathrm{SW}}\sigma}{k_{\mathrm{B}}T} - \frac{2\pi D^{\mathrm{SW}}\eta_{\mathrm{E}}\sigma}{k_{\mathrm{B}}T} = \frac{4yf_{\mathrm{E}}}{25\omega(1 + S)} \tag{19}$$

where η_{E} is the Enskog viscosity arising from uncorrelated binary collisions and η^{SW} is the viscosity for square-well fluids for uncorrelated and correlated binary collision and η_{E} can be determined as

$$\frac{\eta_{\mathrm{E}}}{m\rho} = \sigma^2\omega Y \tag{20}$$

where

$$Y = \left\{\frac{5\sqrt{\pi}}{96yg^{\mathrm{SQ}}(\sigma)}\left(1 + \frac{8yg^{\mathrm{SQ}}(\sigma)}{5}\right)^2 + \frac{8yg^{\mathrm{SQ}}(\sigma)}{5\sqrt{\pi}}\right\} \tag{21}$$

$$S = \frac{f_{\mathrm{E}}}{32\omega} = \frac{yg^{\mathrm{SQ}}(\sigma)}{2\sqrt{\pi}} \tag{22}$$

f_{E} and ω are already defined by eq 4.

To test the validity of our results, a comparison is also made with the theory formulated by Nigra and Evans.[11] The diffusion coefficient (in reduced units) proposed by Nigra and Evans[11] can be solved as

$$D^{*\mathrm{SW}}_{\mathrm{Evans}} = \frac{3}{8\rho^*\sqrt{\pi}}\frac{1}{g^{\mathrm{HS}}(\sigma)[1 + 8y\lambda^3 g_1(\lambda\sigma)f^2F]} \tag{23}$$

where

$$F = \frac{7\lambda^3 + 2}{(42\lambda^3 - 7f\lambda^3 - 8f)}$$

$$f = 1 - \mathrm{e}^{-\varepsilon/kT} = 1 - \mathrm{e}^{-1/T^*}$$

$$g_1(\lambda\sigma) = \mathrm{e}^{\varepsilon/kT} = \mathrm{e}^{1/T^*}$$

The shear viscosity (in reduced unit) proposed by Nigra and Evans[11] can be written as

$$\eta^{*\mathrm{SW}}_{\mathrm{Evans}} = \frac{8\rho^*\sqrt{\pi}}{3}\left(\frac{g^{\mathrm{HS}}(\sigma)}{2\pi} + \frac{4f^2\pi\lambda^5\rho^{*2}g_1(\lambda\sigma)\check{n}}{15}\right) \tag{24}$$

where

$$\eta^{*\mathrm{SW}} = \frac{\eta^{\mathrm{SW}}}{\left(\frac{k_{\mathrm{B}}T}{m\sigma^2}\right)^{1/2}\frac{m}{\sigma}} \tag{25}$$

$$\check{n} = \frac{11\lambda^2 + 4}{11(10 - f)\lambda^5 - 24f} \tag{26}$$

$$\rho^* = \rho\sigma^3$$

The shear viscosity (in reduced units) can be obtained from eq 23 by employing the Stokes−Einstein relation from eq 19.

For 2D fluids, unlike 3D fluids, the Stokes−Einstein relation is lacking and is not well established. However, recently Garcia-Rojo et al.[12] have calculated transport coefficients for hard discs. The self-diffusion coefficient from the Enskog equation in the first Sonine approximation for $d = 2$, that is[13]

$$D^{\mathrm{HD}} = \frac{1}{2\rho\sigma g_1(\sigma)}\left(\frac{k_{\mathrm{B}}T}{\pi m}\right)^{1/2} \tag{27}$$

Here T is the temperature; k_{B} is the Boltzmann constant; σ is the diameter of the hard discs; m is their masses; and $g_1(\sigma)$ is the value of the equilibrium pair correlation function at contact, which is a function of the density ρ.

Three different expressions for the pair correlation function at contact are provided by Henderson,[14] Luding,[15] and Garcia-Rojo et al.[12] However, they do not show any effect on the Stokes−Einstein relation. The results just overlap each other.

The shear viscosity of hard discs is given by[12]

$$\eta^{\mathrm{HD}} = \eta_0\left\{\frac{1}{g_1(\sigma)} + 2y_1 + \left(1 + \frac{8}{\pi}\right)g_1(\sigma)y_1^2\right\} \tag{28}$$

where $y_1 = (\pi/4)\rho\sigma^2$, the packing fraction

$$\eta_0 = \frac{1}{2\sigma}\left(\frac{mk_{\mathrm{B}}T}{\pi}\right)^{1/2}$$

Our aim is to calculate the S−E relation for 2D fluids. The 2D S−E relation is given by[2]

$$D^{\mathrm{HD}} = \frac{k_{\mathrm{B}}T}{C_{2\mathrm{D}}\pi\eta^{\mathrm{HD}}} \tag{29}$$

where $C_{2\mathrm{D}} = 1.69$ as proposed by Liu et al.[2]

Thus, the Stokes−Einstein relation for 2D fluids can be written as

$$\frac{1.69D^{\mathrm{HD}}\eta^{\mathrm{HD}}\pi}{k_{\mathrm{B}}T} = \frac{0.33183}{y_1g_1(\sigma)} \times \left\{\frac{1}{g_1(\sigma)} + 2y_1 + 3.546479{y_1}^2g_1(\sigma)\right\} \tag{30}$$

Result and Discussion

The square-well fluid is the simplest one possessing the basic characteristic of real fluids. In the recent past, several

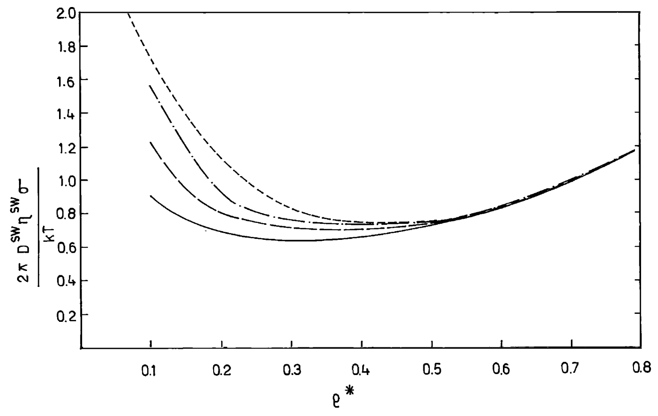

Figure 1. Stokes−Einstein relation for square-well fluids. The solid line is for $T^* = 2$, the big dashed line for $T^* = 3$, and the dash-dotted line for $T^* = 5$, and the small dashed line represents SE relation for a hard sphere system. On the *x*-axis the reduced density and on the *y*-axis the Stokes−Einstein relations are plotted.

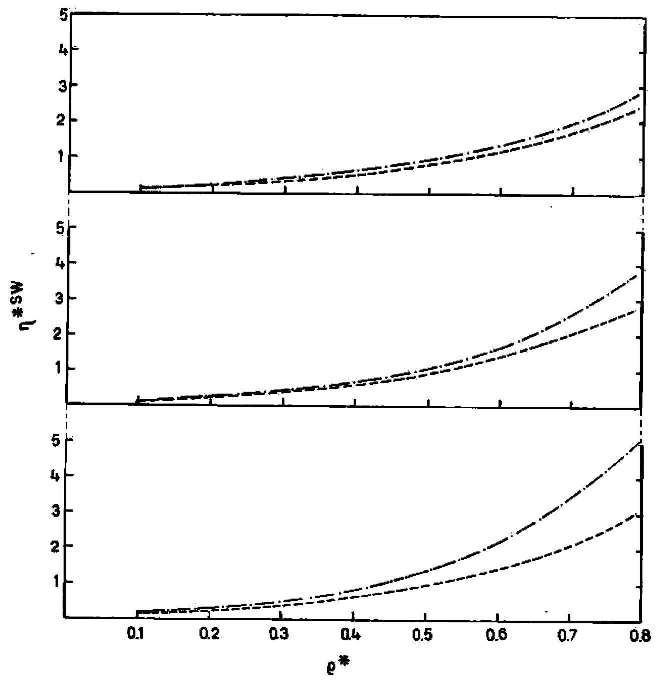

Figure 2. Comparison of the reduced shear viscosity of square-well fluid obtained from the direct expression of shear viscosity and with that obtained by employing the SE relation from the Nigra and Evans model for $T^* = 3$, 2, and 1.5 from top to bottom, respectively. Dotted lines (.....) represent the results from the Nigra and Evans model,[11] and dash dot (•−•−) lines represent the results from the Stokes−Einstein relations. On the *x*-axis the reduced density and on the *y*-axis the reduced shear viscosity are plotted.

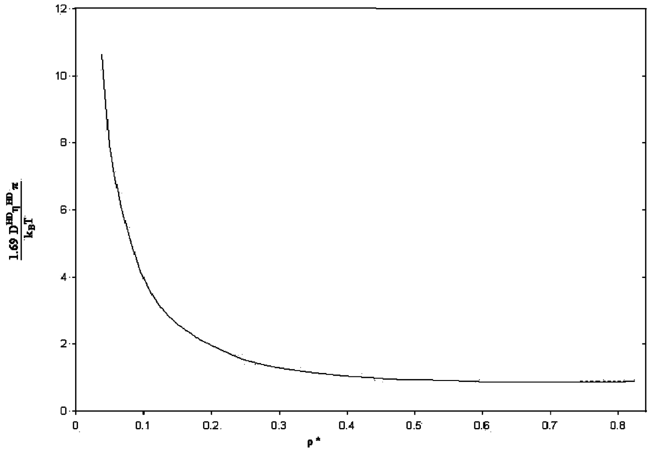

Figure 3. Stokes−Einstein relation for hard discs at different densities. On the *x*-axis the reduced density and on the *y*-axis the Stokes−Einstein relation are plotted.

theories[6,9,16−20] have been developed to establish accurate expressions for the self-diffusion coefficient of the hard sphere system. One such theory is developed by Evans[6] to calculate the velocity time correlation function for a hard sphere system. We apply this approach to calculate self-diffusion coefficient and shear viscosity of square-well fluids and hence the Stokes−Einstein relation. The attractive feature of the square-well fluids in the Chapman−Enskog theory is the radial distribution function at the point of contact, i.e., the radial distribution function at the distance of the centers of the molecules at the moment of a collision for square-well molecules. In the present work, this characteristic feature has been explored by calculating pair correlation function at contact in a high-temperature approximation[21,22] for square-well fluids. The numerical results of the Stokes−Einstein relation are calculated from eq 19. Figure 1 shows the Stokes−Einstein relation for a square-well fluid. Figure 1 predicts that the Stokes−Einstein relation is sharply dependent on the temperature at lower densities, while it tends to unity at higher densities and similar to a hard sphere system in medium and high densities. It is also investigated that at lower densities $[(2\pi\eta^{SW}D^{SW}\sigma)/k_BT]$ tends to deviate to lower values with increasing well depth ε^* (i.e., T^{*-1}). This is in agreement with molecular dynamics results.[23,24] Most of the literature is concerned with the hard sphere system and simply discusses the failure of the Stokes−Einstein at low temperatures and not the variation of the Stokes−Einstein relation with temperature.

To examine the validity of our results for the Stokes−Einstein relation at low temperatures, we have also calculated the shear viscosity directly and with that obtained from diffusion coefficients by employing the Stokes−Einstein relation. Both the expressions of shear viscosity and diffusion coefficient are derived by Nigra and Evans[11] under the same conditions. Two results are compared and presented in Figure 2 for $\lambda = 1.5$ at $T^* = 3$, 2, and 1.5. It is evident from Figure 2 that the shear viscosity obtained by employing the Stokes−Einstein results tends to deviate at low temperatures from the results obtained directly from shear viscosity expression. This deviation shows that the Stokes−Einstein relation fails for low-temperature liquids.

For 3D liquids, the failure of the Stokes−Einstein relation is well-known. For 2D liquids, earlier results suggest that the Stokes−Einstein relation should not be valid at all as the transport coefficients D and η are not valid. Now, it has been shown in several simulation results[25−28] that the shear viscosity coefficient η and diffusion coefficient D are meaningful. Recently, Liu et al.[2] have performed equilibrium molecular dynamic simulations with a Yukawa pair potential. The Stokes−Einstein relation is tested in the regimes $124 < \Gamma < 145$ where motion is diffusive and D is meaningful in 2D liquids. They observed the deviation from linear scaling for $\Gamma > 124$ near the disorder transition that indicates a violation of the Stokes−Einstein relation due to decoupling of diffusive and viscous transport. They found that the diffusion coefficient is larger than would be expected if the S−E relation was valid. We performed the calculation of the S−E relation using eq 30, and the results are shown in Figure 3. It can be seen that the S−E does not remain valid at low densities as also observed for 3D liquids. We have also performed calculations for different expressions of pair correlation functions at contact[14,15,12] However, we have found no change in the plot of the S−E relation as a function of ρ^* despite the fact there is a significant change in the values of the pair correlation function at contact described by the authors of refs 14, 15 and 12. This may be due to the fact that changes in D and η due to different pair correlation functions at contact may nullify each other.

Conclusion

In the present work, it has been shown that the Stokes−Einstein relation fails for square-well fluids at low temperatures. In most of the literature, the failure of the Stokes−Einstein relation has been shown for the hard sphere system. We have investigated that the hard sphere system can be transformed into square-well fluids by employing eq 13. Evans[6] has calculated velocity correlation and diffusion coefficients for hard sphere system, while we have calculated is for square-well fluids. The importance of Figure 1 is that it shows the variation of the Stokes−Einstein relation with temperature for square-well fluids, while in the literature only failure of the Stokes−Einstein relation at low temperature has been predicted for the hard sphere system. To show the changes in the Stokes−Einstein relation from hard sphere to square-well fluids, the hard sphere results are plotted in Figure 1. The Stokes−Einstein relation for square-well fluids may coincide with the Stokes−Einstein relation of hard sphere fluids by raising the temperature when square-well fluid becomes automatically hard sphere fluid.

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