Letters to the Editor

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Transport properties in the mean spherical approximation

R. V. Gopala Rao and T. Nammalvar

Physical Chemistry Section, Jadavpur University, Calcutta-700032

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In this note it is proposed to utilise the analytical expression of $S(K)$, the structure factor, which has been derived recently treating the square well (SW) potential as a perturbation on the hard-core in the mean spherical approximation (Gopala Rao & Nammalvar 1975, 1976) for computing the transport properties of some liquids.

Enskog's equations for transport coefficients of hard spheres do not account for the attractive forces that exist between real molecules and assume only binary collisions. They even fail to predict the density dependence of transport coefficients at density much above the critical value. In the liquid regions the SW model is much preferable for it accounts for the attractive forces that exist between molecules and neglect many body collisions too. The theory based on the SW model has been developed by Davis *et al* (1961). By solving the modified Boltzmann equation they obtained the transport properties for a pure component as follows :

Shear viscosity :

$$\eta = \frac{5}{16\sigma^2}\left(\frac{mkT}{\pi}\right)^{\frac{1}{2}}\left[\frac{\left\{1+\frac{8}{3}\zeta_3(g(\sigma)+\lambda^3 g(\lambda\sigma))\eta\right\}^2}{g(\sigma)+\lambda^2 g(\lambda\sigma)\left[\Xi+\frac{1}{6}\left(\frac{\epsilon}{kT}\right)^2\right]}+\frac{48}{25\pi}(4\zeta_3)^2(g(\sigma)+\lambda^4 g(\lambda\sigma)\Xi)\right]. \quad \ldots (1)$$

Bulk viscosity :

$$K = \frac{16\zeta_3}{\pi\sigma^2}\left(\frac{mkT}{\pi}\right)^{\frac{1}{2}}\eta\, g(\sigma)+\lambda^4 g(\lambda\sigma)\Xi\Big]. \quad \ldots (2)$$

Thermal conductivity :

$$\lambda = \frac{75}{64\sigma^2}\left(\frac{k^3T}{\pi m}\right)^{\frac{1}{2}}\left[\frac{\left\{1 + \frac{12}{5}\zeta_3[g(\sigma) + \lambda^3 g(\lambda\sigma)\psi]\right\}^2}{g(\sigma) + \lambda^2 g(\lambda\sigma)\left[\Xi + \frac{11}{16}\left(\frac{c}{kT}\right)^2\right]}\right.$$

$$\left. + \frac{32}{25\pi}(4\zeta_3)^2(g(\sigma) + \lambda^4 g(\lambda\sigma))\Xi)\right]. \qquad \ldots (3)$$

Self diffusion :

$$D = \frac{3}{8\rho\sigma^2}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}[g(\sigma) + \lambda^2 g(\lambda\sigma)\Xi]^{-1} \qquad \ldots (4)$$

In eqs. (1) through (4) the functions Ξ, ψ and ζ_3 are defined as

$$\Xi = e^{c/KT} - \frac{c}{kT} - 2\int_0^\infty x^2\left(x^2 + \frac{c}{kT}\right)^{\frac{1}{2}} e^{-x^2}dx \qquad \ldots (5)$$

$$\psi = 1 - e^{c/KT} + \frac{c}{2kT}\left(1 + \frac{4}{\sqrt{\pi}}\, e^{c/KT}\int_{(c/kT)^{\frac{1}{2}}}^{\infty} e^{-x^2}x^2dx\right) \qquad \ldots (6)$$

and

$$\zeta_3 = \frac{\pi\rho\sigma^3}{6}. \qquad \ldots (7)$$

Here ρ is the number density, σ is the molecular diameter and the rest of the symbols have their usual significance. The functions in eqs. (5) and (6) have been taken from Luks *et al* (1966).

To obtain the above transport coefficients the values of σ, λ and c also $g(\sigma)$ and $g(\lambda\sigma)$ are needed. In the present calculations σ, λ and c/k_B have been taken from authors' own data where in a satisfactory fit of structure factor has been made (Gopala Rao & Nammalvar 1975, 1976) and are given in Table 1. The values of $g(\sigma)$ and $g(\lambda\sigma)$ have been obtained from the smoothed values of the radial distribution function computed from the structure factor expression.

In this connection we would like to point out that Davis & Luks (1965) in order to calculate the transport properties have used the experimental thermal conductivity values to compute the correlation functions from which they could predict viscosity coefficient and diffusion coefficient for liquid argon over a wide range of temperatures and pressures. They also obtained the transport properties with the numerically computed pair correlation functions $g(\sigma)$ and $g(\lambda\sigma)$. But in the present method the transport properties could be computed without prior

knowledge of one of the coefficients. The values so calculated with these sets of parameters, obtained from static structure factor data, are given in Table 2 and are compared with literature values wherever available (Lin *et al* 1964, Rice *et al* 1964, Palyvos & Davis 1967, Squire *et al* 1953, Gray 1968). The agreement between the calculated and experimental values is satisfactory with the exception of krypton for which calculations have been made near critical temperature. Similar deviation of about 63% has been observed in the case of argon near the critical region (McLaughlin & Davis 1966).

Table 1. Potential paramoters

Substance	T °K	σ Å	ϵ/k °K	λ
Argon[1]	163	3·0	124·6	1·5
	153	,,	,,	,,
	148	,,	,,	,,
	143	,,	,,	,,
Helium[2]	2·4	3·0	5·11	1·05
Methane[3]	186	3·45	148·0	1·5
Krypton[4]	210	3·5	134·5	1·4
Neon[5]	44·2	2·44	35·6	1·5

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2. *Ind. J. Pure & Appl. Phys.* **13**, 464 (1975).
3. —, *Chem. Phys. Lett.* **31**, 113 (1975).
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5. — —, To be published.

Table 2. Transport coefficients

Substance	T °K	$\rho.10^2$ atom/Å^3	$\eta.10^4$ poise		$K.10^4$ poise		$\lambda.10^4$ cal/cm sec °K		$D.10^5$ cm^2/sec	
			cal	exp	cal	exp	cal	exp	cal	exp
Argon	163	1·175	2·01	3·1	1·97	10·4	0·228	0·70	21·7	11·6
	153	1·371	4·64	4·6	8·42	10·0	0·775	1·10	10·71	10·6
	148	1·479	5·18	5·4	7·0	9·8	0·95	1·20	10·52	10·0
	143	1·371	5·52	6·3	7·8	9·6	0·796	1·38	9·27	9·1
Helium	2·4	2·193	2·34	2·75	3·79	—	2·82	4·1	0·58	—
Methane	186	0·9016	2·59	3·38	3·24	–	0·89	2·15	21·4	18·0
Krypton	210	0·75	4·07	37·0	2·12	—	0·3	1·7	0·22	4·5
Neon	44·2	2·0	1·92	– –	2·16	– –	0·59	—	8·6	—

From the satisfactory agreement between calculated and experimental values it can be safely concluded that the SW theory which can be considered as a sub-

stantial improvement over the hard sphere theory of liquids. The use of equilibrium values of $g(\sigma)$ and $g(\lambda\sigma)$ in the evaluation of transport properties can be thought of as an important step in achieving a unified theory of the liquid stat

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Magnetic susceptibility of the free charge carriers in antimony telluride

(Miss) B. Roy, B. R. Chakraborty and A. K. Dutta

Department of Magnetism,
Indian Association for the Cultivation of Science, Calcutta-700032

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The magnetic properties of antimony telluride, (Sb_2Te_3), a typical partially conducting chalcogenide have so far been very sparingly studied. Matyas has studied the magnetic susceptibility of Sb_2Te_3 in the vicinity of its melting point only (Matyas 1971) and in the presence of dopants (Horak *et al* 1975). Kutvitskii *et al* (Kutvitskii *et al* 1970, 1972) have also measured the magnetic susceptibility of Sb_2Te_3 in both solid and molten states. In all these measurements it has been found to be diamagnetic. None of these measurements appear to have been made with single crystals and at different temperatures. We have therefore undertaken to study the principal magnetic susceptibilities $\chi_\perp$ and $\chi_\parallel$