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Transport properties of the fluid for hard convex body

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Abstract : The Isotropic-symmetric and orientational co-relations for hard convex bodies (HCB) model, exhibit simpler behavior in the surface-to-surface than in the more customary centre-to-center co-ordinate representation. The radial wave equation of a HCB's (hard convex bodies) model coordinate system has been described and expressed for the pair intermolecular potential specified in terms of the support function h(x) for the calculation of the phase shifts. The Intermolecular potential for HCB'S reduces to hard sphere (HS) Intermolecular potential for major and minor axis ratio equal to one and has exactly the same surface-to- surface distribution as for HCB's. Thus, the theoretical work supporting the concept that the HCB model would prove to be as valuable as hard sphere model as reference fluid for real fluids.

Keywords : Co-ordinate System, Support function h(x), hard convex fluid and Intermolecular potentia

INTRODUCTION

The phase shifts is the solution of the radial wave equation. The expression for the radial wave equation of a HCB Model co-ordinate system has been described first and expressed for the pair intermolecular potential specified in terms of the support function h(x) and surface -to-surface co-ordinate representation. The Transport properties of the fluid for HCB model may be calculated if one knows the cross section parameter of the transport function. Phase shift is known for HCB model and cross - section has also been expressed in terms of the phase shift, so the cross- section of different transport parameter may be calculated

METHODOLOGY

The support function h(x) is defined as the projection.

$$h(x) = \hat{k}.\rho - -(1)$$

Where $\overset{\Lambda}{\rho}$ is the vector extending from the centre to the point on the surface to the minimum separation

$$\vec{\rho} = \hat{k}\,h(x) + \left(1 - \hat{k}\hat{k}\right).\hat{e}\,h'(X) - -(2)$$

$$X = \hat{K}.\hat{e} = \cos\theta - -(3)$$

Where x defines the orientation of HCB'S and the unit vectors $\overset{\Lambda}{e}$ is the director axis. When x=cos θ=1 the orientation is along semi-major axis "a", when x=cosq =0 the orientation is along semi-minor axis "b".

For the HCB'S with semi-major axis "a" and the semi-minor axis "b", the support function is

$$h(X) = b\left[1 + \in X^2\right]^{1/2} \qquad \text{Where } \in = \left(\frac{a}{b}\right)^2 - 1$$

$$\text{And } h'(X) = \frac{dh(X)}{dX} = \frac{b^2 \in X}{h(X)}$$

The support function h(x) for $\frac{a}{b}$ =1 reduces to a (or a=b), and the intermolecular potential for HCB'S reduces to hard sphere, Intermolecular potential which has exactly the same surface - to -surface distribution as the HCB'S

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The center-to-center distance $\vec{r}(k)$ is

$$\vec{r}(\hat{k}) = \vec{k} + \rho_1\left(\hat{k}\right) - \rho_2\left(-\hat{k}\right)$$

To avoid the over lapping situation the expression for has been $\vec{r}(\hat{k})$ Transformed to

$$\vec{r}(\hat{k}) = \hat{k}\left[k + h(X)\right]$$

With $h(x) = h(x_1) + h(x_2)$

In case of spherical molecules $r(\hat{k})$ reduces to

r = a+k or b+k

In order to make calculations of phase shifts it is necessary to specify the intermolecular potential function in the radial wave equation.

The expression for $\nabla^2\Psi$ in terms of HCB'S co-ordinate system is

$$\left[\begin{array}{l}\frac{1}{(h(x)+K)^2}\frac{\partial}{\partial K}\left\{(h(x)+K)^2\frac{\partial}{\partial K}\right\}+\frac{1}{(h(x)+K)^2\sin\theta}\frac{\partial}{\partial\theta}\\ \left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{(h(x)+K)^2\sin^2\theta}\frac{\partial}{\partial\varphi^2}\end{array}\right]\Psi = \nabla^2\Psi \quad --(4)$$

And,

The radial wave equation may be written in the reduced form

$$\frac{d^2}{dK^{*2}}(K^*\psi(K)) + \left[J^{*2} + \frac{16\pi^2}{\Delta^{*2}}\left(\frac{1}{K^{*12}} - \frac{1}{K^{*6}}\right) - \frac{\ell(\ell+1)}{(1+K^*)^2}\right](K^*\psi(K)) = 0 \quad --(5)$$

Where $K^* = \frac{K}{h(x)}$; $J^* = J\,h(x)$ and $\mu = \frac{m}{2}$,

m is the mass of the particle, μ is the reduced mass and is $\mu = \frac{m_1 m_2}{m_1 + m_2}$ Here $m_1 = m_2$ for identical particle.

$$\Delta^* = \frac{h}{h(x)\sqrt{2E\mu}}$$

or, $\Delta^* = \frac{h}{h(x)\sqrt{Em}}$, is a reduced quantum parameter.

The reduced quantum mechanical parameter

$\Delta^* = \frac{h}{a(mE)^{\frac{1}{2}}}$, when $x = \cos\theta = 1$, the orientation is along semi - major axis 'a' and

$\Delta^* = \frac{h}{b(mE)^{\frac{1}{2}}}$ When $x = \cos\theta = 0$, the orientation is along semi-Minor axis 'b'.

The asymptotic solution of the radial wave equation for real(interacting) and ideal (non-interacting) pairs of molecules are sinusoidal and differ only in the phase of the sine functions, the difference being the phase shifts, η_ℓ (J*). The phase shift depends upon the angular momentum quantum number ℓ and the wave number of relative motion.

The integral expression for phase shifts for the HCB'S model may be written as

$$\frac{16\pi^{\frac{5}{2}}}{\sqrt{2}.J^{*\frac{3}{2}}\Delta^{*2}}\int_0^\infty (1+K^*)^{\frac{1}{2}}.J_{\ell+\frac{1}{2}}(J^*(1+K^*)).$$

$$\eta_\ell = \tan^{-1}\frac{\left(\frac{1}{K^{*12}} - \frac{1}{K^{*6}}\right)\sin\left(J^*(1+K^*) - \frac{\ell\pi}{2}\right)}{1 - \frac{16\pi^{\frac{5}{2}}}{\sqrt{2}.J^{*\frac{1}{2}}\Delta^{*2}}\int_0^\infty (1+K^*)^{\frac{1}{2}}.J_{\ell+\frac{1}{2}}(J^*(1+K^*))\left(\frac{1}{K^{*12}} - \frac{1}{K^{*6}}\right)\cos\left(J^*(1+K^*) - \frac{\ell\pi}{2}\right)} \quad --(6)$$

Thus the effective molecular cross- section for all types of encounter in He^3 is

$$Q(J^*) = \frac{3}{4}Q(J^*)_{F\text{-}D} + \frac{1}{4}Q(J^*)_{B\text{-}E}$$

Where,

$$Q(J^*)_{F.D} = \frac{16\pi}{J^{*2}}\sum_{\ell=odd}\frac{(\ell+1)(\ell+2)}{2(2\ell+3)}\sin^2(\eta_{\ell+2} - \eta_\ell)$$

$$Q(J^*)_{B.E} = \frac{16\pi}{J^{*2}}\sum_{\ell=even}\frac{(\ell+1)(\ell+2)}{2(2\ell+3)}\sin^2(\eta_{\ell+2} - \eta_\ell)$$

The effective cross section for He^4 is given by the expression $Q(J^*)_{B.E}$ only.

For $\frac{a}{b} = 2$, the cross - section have been calculated both for major and minor axis for He^3 and He^4 (table 1, 2, 3 & 4). The graphs for cross section of Helium illustrate the diffraction effects on encountered in transport phenomena are shown in figure 1, 2, 3 & 4.

The cross section for HS model (k, θ, ϕ) have also been calculated table 5 and 6 and their graphs are shown in figure 5 and 6. This has been done for major axis only. Because $\frac{a}{b} = 1$, here.

Table - 1

Cross - section of He^3 along major axis	
J*	**R(J*) =**
0.5	216.863
0.6	134.604
0.7	88.284
0.8	60.252
0.9	42.767
1	30.652

J*	R(J*) =
1.1	23.801
1.2	16.801
1.3	11.541
1.4	8.527
1.5	6.994
1.6	5.907
1.7	4.797
1.8	3.63
1.9	2.535
2	1.671

Table - 2

Cross - section of He^4 along major axis

J*=	Q(J*)
0.2	483.451
0.3	1.291.103
0.4	477.754
0.5	349.773
0.6	286.841
0.7	236.564
0.8	191.014
0.9	148.295
1	103.586
1.1	70.226
1.2	36.801
1.3	15.915
1.4	5.932
1.5	1.976
1.6	0.578
1.7	0.136
1.8	0.024
1.9	0.022
2	0.19

Table - 3

Cross - section of He^3 along minor axis

J*	R(J*) =
0.5	266.03
0.6	158.718
0.7	100.481
0.8	68.832
0.9	50.597
1	39.751
1.1	34.438
1.2	31.479
1.3	30.112
1.4	29.174
1.5	27.227
1.6	22.445
1.7	16.232
1.8	12.66
1.9	11.076
2	9.888

Table - 4

Cross - section of He^4 along minor axis

J*=	Q(J*)
0.1	320.817
0.2	339.975
0.3	406.502
0.4	656.722
0.5	547.205
0.6	365.879
0.7	282.426
0.8	230.03
0.9	190.105
1	156.317
1.1	132.703
1.2	111.273
1.3	92.892
1.4	73.535
1.5	48.566
1.6	22.388

Table - 5

Cross - section of He^3 for HS Model

J*	R(J*) =
0.5	415.88
0.6	270.155
0.7	189.99
0.8	142.521
0.9	112.387
1	92.059
1.1	77.631
1.2	66.95
1.3	58.759
1.4	52.288
1.5	47.04
1.6	42.689
1.7	39.007
1.8	35.837
1.9	33.065
2	30.609

Table - 6

Cross - section of He^4 for HS Model

J*=	Q(J*)
0.1	39.611
0.2	39.02
0.3	38.408
0.4	37.761
0.5	37.069
0.6	36.32
0.7	35.526
0.8	34.67
0.9	33.757
1	32.787
1.1	31.765
1.2	30.693
1.3	29.579
1.4	28.43
1.5	27.254
1.6	26.06

Cross-Section of He^3 along major axis

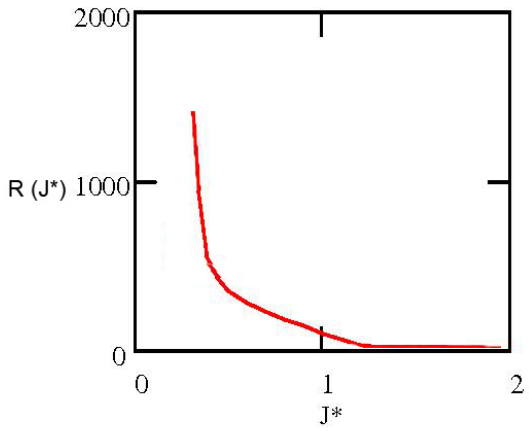

Figure -1

Cross-Section of He^4 along major axis

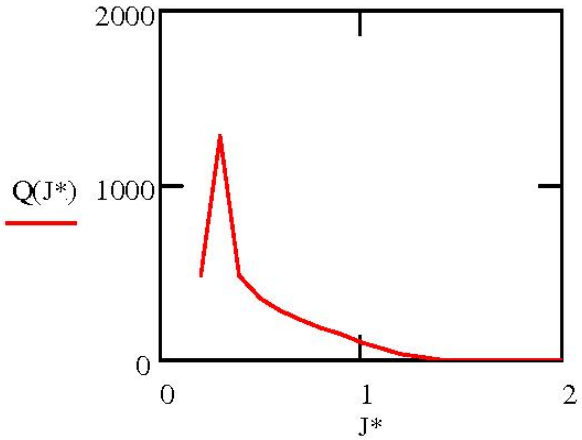

Figure -2

Cross-Section of He^3 along minor axis

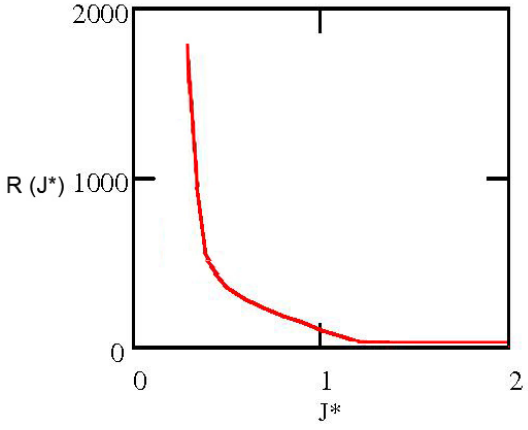

Figure -3

Cross-Section of He^4 along minor axis

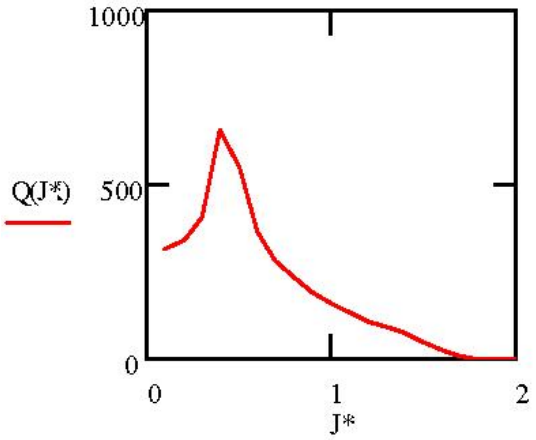

Figure -4

Cross-Section of He^3 for HS Model

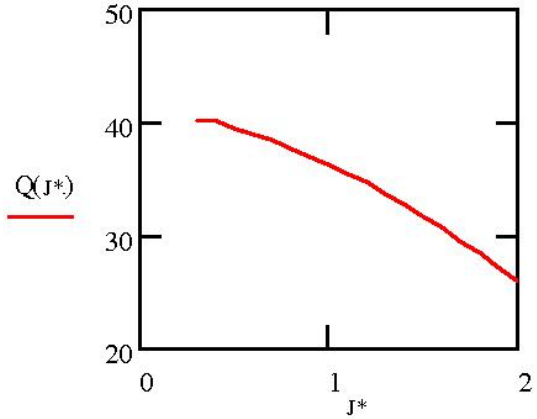

Figure -5

Cross-Section of He^4 for HS Model

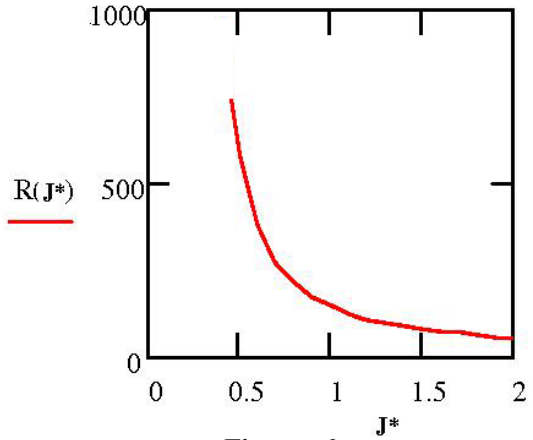

Figure -6

RESULT AND DISCUSSION

These results for the cross section have been plotted in figures for comparison also. The most important difference result from the different behavior of h_l for small J* for the case of He^3 and He^4. Q (J*) for He^4 becomes finite for minor axis and infinite for major axis where as Q (J*) for He3 approaches to infinite for J* $\rightarrow$ 0 for HCB model case. This behavior repeated in case of HS model for (k, θ, ϕ) co-ordinate representation for both He^4 and He^3.

CONCLUSION

The theoretical work supporting the concept that the HCB model would prove to be as valuable as hard sphere model as a reference fluid for real fluids. Thus the proposed radial wave equation based on the surface-to-surface distance K and the potential defined in terms of the support function h(x) simplifies the determination of phase shift and cross-section for HCB'S model. The calculated cross-section values of He^4 and He^3 may be used for the calculation of the transport properties

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