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STUDY OF RADIAL WAVE EQUATION IN TERMS OF HCB MODEL

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Abstract- The Phase shifts needed for the calculation of the transport properties of hard convex body (HCB) fluid in quantum mechanics is the solution of the radial wave equation described by the HCB coordinate systems. The radial wave equation described by HCB-coordinate system has been deduced and expressed for the pair intermolecular potential specified in terms of the support function h(x) and surface-to-surface" coordinate representation. The radial wave equation has been expressed in the reduced form.

Keywords- Radial wave equation, HCB Coordinate System, Phase Shift, Support Functions.

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Introduction

In quantum mechanical calculation of the transport phenomena, the major problem is the evaluation of the Radial wave equation. 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 "K" co-ordinate representation. The properties of hard convex bodies (HCB's) necessary for our analysis are due to Kihara [1].

Analysis of Ñ ²Y in Terms of HCB Co-Ordinate

Let us first assume that the convex body has a smooth surface and that each supporting plane has a contact of first order with the convex body. Let r (q, f) be the radius vector from the origin to the contact point of the body with the supporting plane in the direction (q, f).

Then by use of the unit vector $\hat{K}$ (q, f) in the direction (q, f) so, the identity

$$X = (h(x)+K)\sin\theta\cos\phi$$

$$Y = (h(x)+K)\sin\theta\sin\phi$$

$$Z = (h(x)+K)\cos\theta$$

Thus for, the expression for Ñ²Y in terms of the above identities, it is desirable to use the procedure for making the transformation from Cartesian coordinates to the required coordinate system. This is done by using the concept of orthogonal curvilinear co-ordinates.

The expression for Ñ²Y (Laplacian) in orthogonal curvilinear coordinates is given by

$$\nabla^2\Psi = \nabla.\nabla\Psi = \frac{1}{h_1h_2h_3}\left[\begin{array}{l}\frac{\partial}{\partial u_1}\left(\frac{h_2h_3}{h_1}\frac{\partial\Psi}{\partial u_1}\right)+\frac{\partial}{\partial u_2}\left(\frac{h_1h_3}{h_2}\frac{\partial\psi}{\partial u_2}\right)\\ +\frac{\partial}{\partial u_3}\left(\frac{h_1h_2}{h_3}\frac{\partial\psi}{\partial u_3}\right)\end{array}\right] \quad (1)$$

where u_1 , u_2 and u_3 are called orthogonal curvilinear co-ordinates and h_1,h_2 and h_3 are called scale factors.

In terms of HCB'S co-ordinates

and $h_1 = 1$

$$h_2 = h(x)+K$$

$$h_3 = \{h(x)+K\}\sin\theta$$

The expression for in terms of HCB'S co-ordinate system is

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

The radial wave equation described by the HCB co-ordinate system is obtained from the [Eq-2] by the method of separation of variables. This method results the expression in one variable.

The Schrodinger eqation for two particles interacting according to a potential function f (k), may be written as

$$\frac{-\hbar^2}{2\mu}\left(\nabla^2\Psi\right)+\phi(K)=E\,\Psi \tag{3}$$

in which E is the total energy of the system.

$$E=\frac{1}{2}\mu g^2 \tag{4}$$

g being the relative speed of the colliding pair before the collision take place and μ is the reduced mass. If we define J by J = μ g, the Schrodinger equation assumes the form [2]

$$\nabla^2\Psi+\left(J^2-\frac{2\phi(K)\mu}{\hbar^2}\right)\Psi=0 \tag{5}$$

$$\left[\frac{1}{(h(x)+K)^2}\frac{\partial}{\partial K}\left\{(h(x)+K)^2\frac{\partial}{\partial K}\right\}+\frac{1}{(h(x)+K)^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{(h(x)+K)^2\sin\theta}\frac{\partial}{\partial\theta}\right]\Psi$$
$$+\left(J^2-\frac{2\phi(K)\mu}{\hbar^2}\right)\Psi=0 \tag{6}$$

This equation will be solved by the method of separation of variables by putting

$$\Psi=\Psi(K)\,\Upsilon(\theta,\phi) \tag{7}$$

Where Y(q, f) are the spherical harmonics and Y(K) satisfy the radial wave equation.

Substituting [Eq-7] into [Eq-6] and dividing by Y and multiplying by $[h(x) + k]^2$ the [Eq-6] becomes

$$\frac{1}{\Psi(K)}\frac{1}{(h(x)+K)^2}\frac{\partial}{\partial K}(h(x)+K)^2\frac{\partial\Psi(K)}{\partial K}$$
$$+\frac{1}{\Upsilon}\left[\frac{1}{(h(x)+K)^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Upsilon}{\partial\theta}\right)+\frac{1}{(h(x)+K)^2\sin^2\theta}\frac{\partial\Upsilon^2}{\partial\phi^2}\right]$$
$$+\left(J^2-\frac{2\phi(K)\mu}{\hbar^2}\right)=0=-\frac{1}{\Upsilon}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Upsilon}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial\Upsilon^2}{\partial\phi^2}\right]=0 \tag{8}$$

The left side of [Eq-8] depends only on K, and the right side depends only on θ and φ, both sides must be equal to a constant that is -*l*(*l*+1).

Thus [Eq-8] gives us a radial equation

$$\frac{1}{(h(x)+K)^2}\frac{\partial}{\partial K}(h(x)+K)^2\frac{\partial\Psi(K)}{\partial K}+$$
$$\left(J^2-\frac{2\phi(K)\mu}{\hbar^2}-\frac{l(l+1)}{(h(x)+K)^2}\right)\Psi(K)=0 \tag{9}$$

The radial [Eq-9], with the change of dependent variable $\Psi(K)=\frac{u(K)}{K}$, becomes

$$\frac{d^2u(K)}{dK^2}+\left(J^2-\frac{2\phi(K)\mu}{\hbar^2}-\frac{l(l+1)}{(h(x)+K)^2}\right)u(K)=0 \tag{10}$$

Where u (k) satisfies the [Eq-10].

The expression for Intermolecular pair potential [3] for HCB Model,

$$\phi(k)=4E\left[\left(\frac{h(x)}{K}\right)^{12}-\left(\frac{h(x)}{K}\right)^{6}\right]$$

the radial wave [Eq-10] may be written in the reduced form

$$\frac{d^2}{dK^2}\left(K^*\Psi(K)\right)+\left[J^{*2}+\frac{16\pi^2}{\Delta^{*2}}\left(\frac{1}{K^{*12}}-\frac{1}{K^{*6}}\right)-\frac{l(l+1)}{(1+K^*)^2}\right]\left(K^*\Psi(K)\right)=0 \tag{11}$$

Where

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

$\mu=\frac{m_1m_2}{m_1+m_2}$, Here m_1= $m_2$for identical particle.

$\Delta^*=\frac{h1}{h(x)\sqrt{2E\mu}}$

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

The reduced quantum mechanical parameter

$\Delta^*=\frac{h}{a(mE)^{\frac{1}{2}}}$,

when x = cosq = 1, the orientation is along semi - major axis 'a' and

$\Delta^*=\frac{h}{b(mE)^{\frac{1}{2}}}$,

when x = cosq = 0, the orientation is along semi minor axis 'b'.

Result and Discussion

Most of the phase shifts given by de Boer and Co-workers for hard sphere model were determined [4] by numerical method integration of the one-dimensional radial Schrodinger equation with the Lennard-Jones Potential. The Phase shifts used for the calculation of the Virial coefficients at very low temperatures. The cross sections for diffusion, for viscosity and thermal conductivity can be determined for HCB Model.

Conclusion

The proposed radial wave equation based on the surface-to-surface distance K and the Potential defined in temrs of the support function h(x) simplifies the determination of phase shift.

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