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COMPARATIVE STUDY OF PHASE SHIFTS FOR HCB MODEL AND HS MODEL

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Abstract- The intermolecular potential for HCB's (hard convex bodies) 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. The radial wave equation reduces to HS Model expression in terms of the surface-to-surface co-ordinate representation. The phase shifts for HS Model have also been calculated.

Keywords- Phase shifts, HCB & HS Model, Co-ordinate System, Support function h(x), Intermolecular potential, radial wave equation, Constant parameters.

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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 phase shifts have been calculated for many values of the quantum number l and J* for the orientation along major and minor axis of HCB Model. The properties of hard convex bodies (HCB's) necessary for our analysis are due to Kihara [1] and others [2].

The phase shifts expression for HCB's model reduces to hard sphere (HS) Model expressions in terms of surface-to-surface co-ordinate representation for the isotropic-symmetric orientation and for major and minor axis ratio equal to one. The phase shifts for HS Model also have been calculated.

Methodology

The essential task is determing the explict form of is that of determining the scale factors.

The condition for this transformation is that the jacobian

$$J = \det \begin{vmatrix} \frac{\partial x}{\partial u_1} & \frac{\partial x}{\partial u_2} & \frac{\partial x}{\partial u_3} \\ \frac{\partial y}{\partial u_1} & \frac{\partial y}{\partial u_2} & \frac{\partial y}{\partial u_3} \\ \frac{\partial z}{\partial u_1} & \frac{\partial z}{\partial u_2} & \frac{\partial z}{\partial u_3} \end{vmatrix}$$

is non zero.

In terms of HCB'S co-ordinates (K,θ,ϕ)

$$u_1 = K, u_2 = \theta, u_3 = \phi$$

and h1 =1

h2 = h(x) + K

h3 = {h(x) + K} sinq

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

$$\left[\frac{1}{(h(x)+K)^2}\frac{\partial}{\partial K}\left\{(h(x)+K)^2\frac{\partial}{\partial K}\right\}+\frac{1}{(h(x)+K)^2\sin\theta}\frac{\partial}{\partial\theta}\right.$$

$$\left.\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{(h(x)+K)^2\sin^2\theta}\frac{\partial}{\partial\theta^2}\right]\psi=\nabla^2\psi \quad (1)$$

The support function h (x) for a/b = 1 reduces to a = b and the intermolecular potential for HCB'S reduces to HS (Hard Sphere) intermolecular potential in terms of surface-to-surface co-ordinate representation.

If h(x) + k is replaced by a + k, this will be corresponds to the co-ordinate r or r = a + k which is a centre-to-centre co-ordinate representation. The phase shift calculated for the major axis for HCB model will corresponds to the phase shift for HS model with radius parameter a.

Result and Discussion

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,hl (J*). The phase shift depends upon the angular momentum quantum number l and the wave number of relative motion.

It is in general not possible to give an exact solution of the radial wave equation for the phases. The expression for the phase shifts has been given by N.F. Mott [3] and applied by Hulthen to calculate hl for different potentials which gives very satisfactory results [4,5].

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

$$Sin\eta_{\ell} = \left(\frac{\pi}{2J^{*}}\right)^{1/2} \int_{0}^{\infty} \left(1+K^{*}\right)^{\frac{1}{2}} J_{\ell+\frac{1}{2}}\left(J^{*}\left(1+K^{*}\right)\right) \frac{16\pi^{2}}{\Delta^{*2}} \cdot \left(\frac{1}{K^{*12}} - \frac{1}{K^{*6}}\right) \cdot \frac{1}{J^{*}} \sin(J^{*}.(1+K^{*}) - \frac{\ell\pi}{2} + \eta_{\ell}) dK^{*} \quad (2)$$

where,

$J_{\ell+\frac{1}{2}}\left(J^{*}(1+K^{*})\right)$ is a Bessel's function [10] given by the expression.

$$J_{\ell+\frac{1}{2}}\left(J^{*}(1+K^{*})\right) = \left[\frac{2}{\pi J^{*}(1+K^{*})}\right]^{\frac{1}{2}} \cdot \left[\sin\left(J^{*}(1+k^{*}) - \frac{\ell\pi}{2}\right) \cdot \sum_{n=0}^{n\le\frac{1}{2}} \frac{(-1)^{n}(\ell+2n)!}{(2n)!\ (\ell-2n)!\ \left(2(k^{*}+1)J^{*}\right)^{2n}} + \cos\left(J^{*}(1+k^{*}) - \frac{\ell\pi}{2}\right) \sum_{n=0}^{n\le\frac{1}{2}(\ell-1)} \frac{(-1)^{n}(\ell+1+2n)!}{(2n+1)!\ (\ell-2n-1)!\ \left(2(k^{*}+1)J^{*}\right)^{2n+1}}\right] \quad (3)$$

the expression (2) may be written as

$$\eta_{\ell} = \tan^{-1} \frac{\left(\frac{1}{K^{*12}} - \frac{1}{K^{*6}}\right) \sin\left(J^{*}\left(1+K^{*}\right) - \frac{\ell\pi}{2}\right)}{1 - \frac{16\pi^{\frac{5}{2}}}{\sqrt{2}J^{*3/2}\Delta^{*2}} \int_{0}^{\infty} \left(1+K^{*}\right)^{\frac{1}{2}} \cdot J_{\ell+\frac{1}{2}}\left(J^{*}(1+K^{*})\right) \cdot \left(\frac{1}{k^{*12}} - \frac{1}{K^{*6}}\right) \cos(J^{*}\left(1+K^{*}\right) - \frac{\ell\pi}{2})} \quad (4)$$

The expression (4) gives the phase shifts corresponding to the angular momentum quantum number l. The expressions for phase shifts corresponding to l = 0,1,2,3,..... have been given in terms of atan {A (J*) }, atan {B (J*) },..... for the calculation with the help of computer.

The expression (4), for example for l = 4, can be written as

$$\int_{a}^{b} z \frac{1}{J^{*2}} \left(\frac{1}{K^{*12}} - \frac{1}{K^{*6}}\right) \cdot \left[\sin\left(J^{*}(1+K^{*}) - 2\pi\right) \cdot \left(1 - \frac{45}{J^{*2}(1+K^{*})^{2}} + \frac{105}{J^{*4}(1+K^{*})^{4}}\right) + \cos\left(J^{*}(1+K^{*}) - 2\pi\right) \cdot \left(\frac{10}{J^{*}(1+K^{*})} - \frac{105}{J^{*3}(1+K^{*})^{3}}\right)\right] \cdot$$

h4 = a tan {E (J*)} =

$$-2\pi) \cdot \left(1 - \frac{45}{J^{*2}(1+K^{*})^{2}} + \frac{105}{J^{*4}(1+K^{*})^{4}}\right) + \cos\left(J^{*}(1+K^{*}) - 2\pi\right) \cdot \left(\frac{10}{J^{*}(1+K^{*})} - \frac{105}{J^{*3}(1+K^{*})^{3}}\right) \cdot \cos\left(J^{*}(1+K^{*}) - 2\pi\right) dK$$

Where

$$J_{4+\frac{1}{2}}\left(J^{*}(1+K^{*})\right) = \left(\frac{2}{\pi J^{*}(1+K^{*})}\right)^{\frac{1}{2}} \cdot \left[\sin\left(J^{*}(1+K^{*}) - 2\pi\right) \cdot \left(1 - \frac{45}{J^{*2}(1+K^{*})^{2}} + \frac{105}{J^{*4}(1+K^{*})^{4}}\right) \cdot + \cos(J^{*}(1+K^{*}) - 2\pi) \cdot \left(\frac{10}{J^{*}(1+K^{*})} - \frac{105}{J^{*3}(1+K^{*})^{3}}\right)\right]$$

and

$$z = \frac{16\pi^{2}}{\left[\frac{h}{S \cdot (mE)^{1/2}}\right]^{2}}$$

The constant parameter a, b and E of the pair potential are known [4]. These values are a = 2.792 x 10-8 cm b = 1.396 x 10-8cm and E =1.414 x 10-15 erg. for ratio a/b = 2. These values have been used here for the calculation of the phase shifts.

This expression for phase shift may be used for the calculation of phase shift along any orientation, this has been used only for major and minor axis orientation here. S is a minor or major axis.

The expression (4) has been used for the calculation of phase shifts for HCB'S model along the major and minor axis for He^{4} and He^{3}. The phase shift with even l (l = 0,2,4,6,.....) have been calculated for He^{4}, since He^{4} has an even number of nucleons and electrons and zero spin. For He^{3} which has an odd number of nucleons and elecrons and spin. The phase shift with both for odd l (l = 0,1,3,5,7,.....) and even l (l = 0,2,4,.....) have been calculated. The calculation of phase shifts have been done with the help of computer for J = 0.1,0.2,..... 2 for each value of l.

The phase shifts have been plotted against the collision energy J* for both orientation in [Fig-1], [Fig-2], [Fig-3], [Fig-4], [Fig-5], [Fig-6].

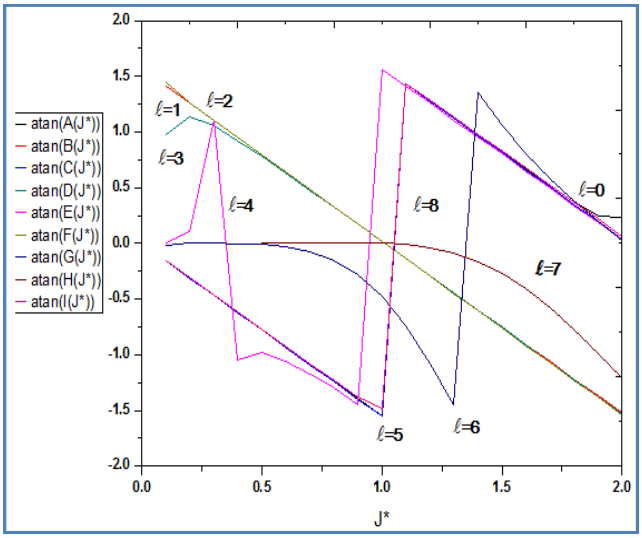

Fig. 1- Phase shift of He^3 along major axis for HCB Model

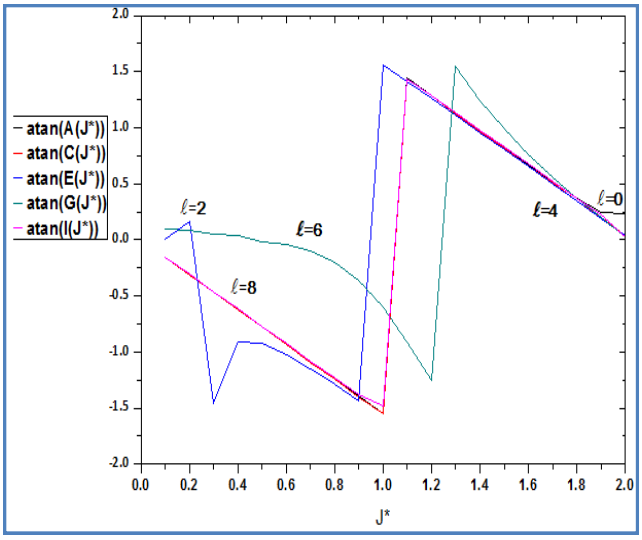

Fig. 2- Phase shift of He^4 along major axis for HCB Model

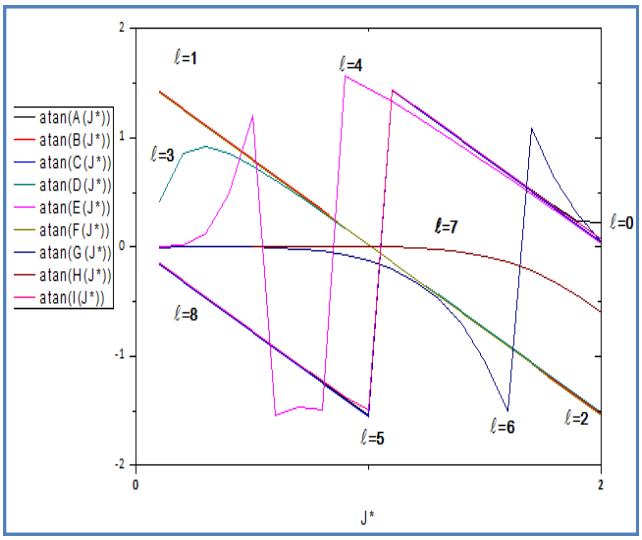

Fig. 3- Phase shift of He^3 along minor axis for HCB Model

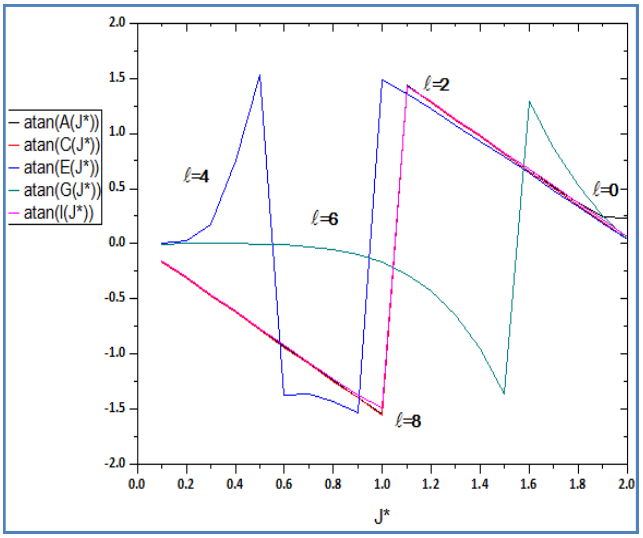

Fig. 4- Phase shift of He^4 along minor axis for HCB Model

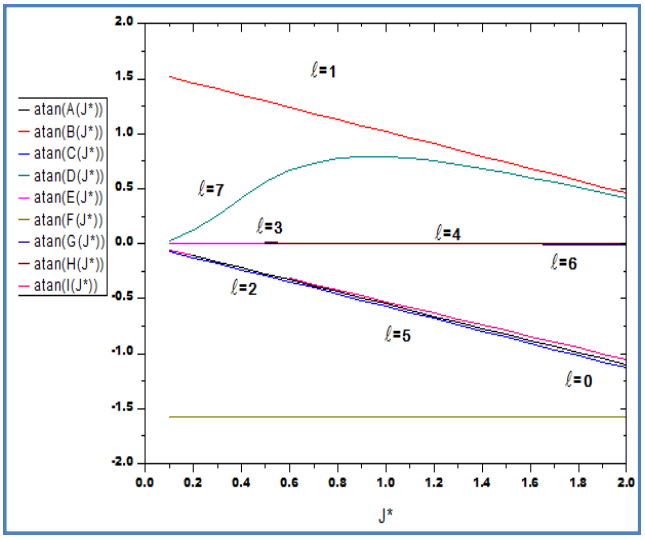

Fig. 5- Phase shift of He^3 for HS Model

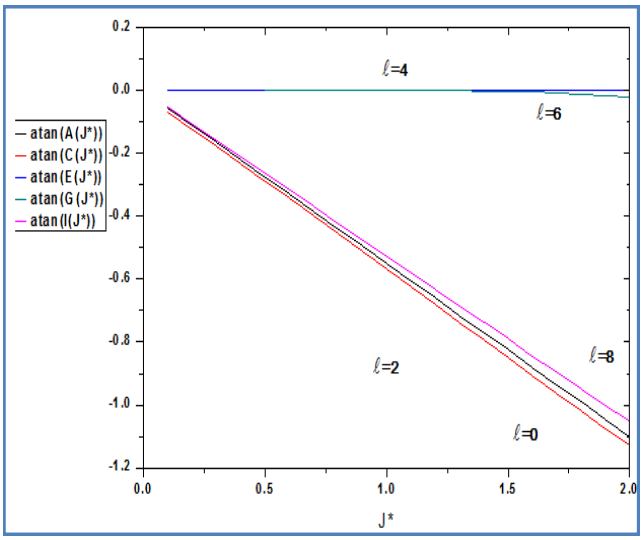

Fig. 6- Phase shift of He^4 for HS Model

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