ANGULAR DISTRIBUTIONS IN THE ELASTIC SCATTERING AND ROTATIONAL EXCITATION OF MOLECULAR HYDROGEN BY ATOMIC HYDROGEN

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ABSTRACT

The effective close-coupling method of Rabitz is tested and used to calculate the angular distributions of the elastic and inelastic scattering of molecular hydrogen in collision with atomic hydrogen when rotational transitions may occur. The interaction potential adopted is the Porter-Karplus semi-empirical potential surface, which was joined smoothly to the correct long-range potentials. Explicit calculations are reported for the differential elastic and total inelastic cross sections in the energy range from 0.1 to 1.5 eV.

Subject headings: atomic and molecular processes — interstellar matter

I. INTRODUCTION

Data on H_2 molecules from the *Copernicus* satellite (Spitzer *et al.* 1973) showed that considerable excitation of the higher rotational levels $j = 4, 5, 6$ of the ground electronic and vibrational state of the H_2 molecule is attained in some interstellar clouds. The observed column densities N_j correspond to rotational temperatures greater than 200 K, considerably higher than the temperatures near 80 K deduced both from the lower rotational levels in H_2 and from 21-cm absorption-line studies (Hughes, Thompson, and Colvin 1971; Radhakrishnan *et al.* 1972; Spitzer *et al.* 1973; Spitzer, Cochran, and Hirshfeld 1974).

It has been conjectured (Spitzer and Zweibel 1974) that the newly formed H_2 molecules leave the grains with a considerable amount (~ 3 eV) of translational kinetic energy. This initial kinetic energy could provide an important heating source for the interstellar gas.

Our main concern in this paper is to present a detailed angular distribution analysis for the (H, H_2) collision system in the energy region greater than 0.5 eV. These data are important in the understanding of the heating mechanism of interstellar clouds by hot H_2 .

Earlier treatments of the rotational inelastic scattering of (H, H_2) include the distorted-wave calculations of Dalgarno, Henry, and Roberts (1966) and of Tang (1969); and the coupled-equation treatment of Allison and Dalgarno (1967), of Hayes, Wells, and Kouri (1971), and of Wolken, Miller, and Karplus (1972). Tang and Karplus (1968) have also studied the elastic scattering problem by using the distorted-wave approximation. In the present study, we shall use the effective close-coupling method introduced by Rabitz (1972) in the form described by Zarur and Rabitz (1974).

II. SCATTERING THEORIES AND THE INTERACTION POTENTIAL

The advantage of the effective close-coupling method of Rabitz (1972) is a substantial reduction in the number of coupled equations, which is accomplished by the construction of an optical potential which eliminates the dependence on the degenerate projection quantum numbers m_j . In order to justify the reliability of the method, we shall employ also the conventional close-coupling theory (Arthurs and Dalgarno 1960). Both theories for rotational excitations have been discussed in detail elsewhere (Chu and Dalgarno 1975*a*) and need not be elaborated here.

The interaction potential we chose to use is the Porter-Karplus (PK) semi-empirical surface (Porter and Karplus 1964). This potential surface was expanded into a series of Legendre polynomials (Wolken *et al.* 1972),

$$V(r, R, \theta) = \sum_{\lambda=0}^{\infty} v_{\lambda}(r, R) P_{\lambda}(\cos \theta), \quad (1)$$

where r and R denote the internuclear vector of H_2 and the channel vector, and $\cos \theta = \hat{r} \cdot \hat{R}$. The $v_{\lambda}(r, R)$ can be computed from the formula

$$v_{\lambda}(r, R) = \frac{2\lambda + 1}{2} \int_{-1}^1 P_{\lambda}(\cos \theta) V(r, R, \theta) d(\cos \theta). \quad (2)$$

In order to obtain the interaction appropriate to pure rotation transitions in the lowest vibrational level $v = 0$, the potential $V(r, R, \theta)$ is averaged over the

$v = 0$ vibrational wave functions. Equation (1) becomes

$$v(R, \theta) = \sum_{\lambda=0}^{\infty} v_{\lambda}(R) P_{\lambda}(\cos \theta), \tag{3}$$

where

$$v_{\lambda}(R) = \int_0^{\infty} dr [u_{00}(R)]^2 v_{\lambda}(r, R),$$

$u_{00}(r)$ being the ground vibrational ($v = 0$) and rotational ($j = 0$) wave function for H_2 . The $v_{\lambda}(R)$ have been evaluated by Wolken *et al.* (1972) for $\lambda = 0, 2, \dots, 12$. The higher order nonspherical terms with $\lambda > 2$ contribute over only a very limited region, and v_0 and v_2 dominate the scattering.

The PK surface, while providing a reasonably accurate description of $H + H_2$ near the saddle-point region, decays to zero exponentially with large R , and does not have the correct long-range C_6/R^6 van der Waals behavior. To ensure the correct asymptotic behavior, we use the potential of Dalgarno, Henry, and Roberts (1966) for values of R larger than its point of intersection with the potential of Porter and Karplus (1964). The potentials of Dalgarno *et al.* are given by

$$v_0(R) = 511.088 \exp(-1.9R) - 251.546/R^6,$$

and

$$v_2(R) = 346.664 \exp(-2.0R) - 27.8767/R^6, \tag{4}$$

where v_{λ} are in units of eV and R in a_0 . Thus the modified surface has three regions: for $R \leq 4.6a_0$, the Porter-Karplus surface is appropriate; for $4.6a_0 \leq R \leq 7.0a_0$, $v_0(R)$ is given by equation (4) and $v_{\lambda}(\lambda > 0)$ are obtained from the Porter-Karplus surface; and for $R \leq 7.0a_0$, $v_{\lambda}(\lambda > 2) = 0$ and v_0 and v_2 are obtained from equation (4).

III. NUMERICAL CALCULATIONS

The Porter-Karplus surface uses a Morse curve with a specific choice of parameters for the potential of an isolated H_2 molecule:

$$v(\text{Morse}) = 4.7466(\text{eV}) \exp[-\alpha(R - R_0)] \times \{\exp[-\alpha(R - R_0)] - 2.0\}, \tag{5}$$

where $\alpha = 1.04435$, $R_0 = 1.40083$, and R is measured in a_0 . In order that the calculation be internally consistent, we have used the energy levels associated with the Morse curve (Wolken *et al.* 1972).

The coupled differential equations associated with both the close-coupling (CC) and effective close-coupling (ECC) methods were solved using the Numerov algorithm (Allison 1970). The scattering matrices thus obtained can be used to calculate the differential, total, diffusion, and viscosity cross sections, after proper account has been taken of the detailed balance relation (Zarur and Rabitz 1974; Chu and Dalgarno 1975*b*).

IV. RELIABILITY OF THE EFFECTIVE CLOSE-COUPPLING METHOD

In a recent paper (Chu and Dalgarno 1975*b*), we have examined the range of applicability of the ECC method, with the conclusion that the ECC method should be satisfactory provided that the anisotropy of the potential is not strong and the impact energy is not close to the rotational threshold. For the system $H + H_2$, all the nonspherical potentials $v_{\lambda}(R)$ ($\lambda \geq 2$) are much smaller than the spherical potential $v_0(R)$ (Wolken *et al.* 1972), and the first condition is met. To explore the severity of the second condition, we carried out close-coupling calculations at an energy of 0.1 eV, which is about twice the threshold for exciting the $j = 0$ to $j' = 2$ transition.

The results of the CC and ECC calculations at $E = 0.1$ eV are summarized in Tables 1 and 2. Table 1 presents the comparison of the total, diffusion, and viscosity cross sections. The agreement between the two sets of calculations is encouraging. In Table 2 we compare the elastic differential cross sections for the transition

The agreement between $(d\sigma/d\Omega)_{\text{CC}}$ and $(d\sigma/d\Omega)_{\text{ECC}}$ is again excellent, not only in the oscillatory structure but also in the absolute magnitude for scattering angles $\theta < 150^\circ$. For $\theta \geq 150^\circ$, the backward scattering region, $(d\sigma/d\Omega)_{\text{ECC}}$ is slightly out of phase. However, this has no significant influence on astrophysical applications, because the magnitude of $d\sigma/d\Omega$ in the backward region is small in comparison with the forward scattering.

TABLE 1
COMPARISON OF TOTAL, DIFFUSION, AND VISCOSITY CROSS SECTIONS OBTAINED FROM CC AND ECC CALCULATIONS AT $E = 0.1$ eV*

$j \rightarrow j'$	TOTAL		DIFFUSION		VISCOSITY	
	CC	ECC	CC	ECC	CC	ECC
0 $\rightarrow$ 0.....	44.9	45.3	16.1	16.6	14.5	14.8
0 $\rightarrow$ 2.....	0.52	0.42	...	...	...	...
2 $\rightarrow$ 0.....	0.18	0.15	...	...	...	...
2 $\rightarrow$ 2.....	47.0	47.8	...	...	...	...

* In units of σ (10^{-16} cm²).

TABLE 2
COMPARISON OF THE ELASTIC DIFFERENTIAL
CROSS SECTIONS FOR THE TRANSITION
 $H + H_2(j = 0) \rightarrow H + H_2(j' = 0)$ AT
 $E = 0.1$ eV IN THE CC AND ECC
FORMALISMS

SCATTERING ANGLE, θ (degrees)	$d\sigma/d\Omega$ (10^{-16} cm 2)	
	CC	ECC
0.....	447	444
5.....	384	284
10.....	56.1	55.7
15.....	55.1	49.7
20.....	11.7	11.9
25.....	3.8	3.6
30.....	5.0	5.4
35.....	3.0	3.7
40.....	3.2	3.5
45.....	3.5	3.6
50.....	2.6	2.8
55.....	3.0	3.1
60.....	2.4	2.2
70.....	2.1	1.8
80.....	1.7	1.7
90.....	1.4	1.7
100.....	1.3	1.3
110.....	1.2	1.1
120.....	0.9	1.2
130.....	0.9	0.9
140.....	0.8	0.8
150.....	0.7	0.9
160.....	0.8	0.6
170.....	0.5	0.9
180.....	1.1	0.3

Although the Porter-Karplus potential surface has been expanded into a series of Legendre polynomials (eqs. [1] and [3]) up to $\lambda = 12$ (Wolken *et al.* 1972), the contribution of v_λ , for which $\lambda > 2$, to the scattering is very small. Table 3 contains the results of ECC calculations at 0.5 eV for the two potentials $V = v_0 + v_2P_2$ and $V = v_0 + v_2P_2 + v_4P_4 + v_6P_6$. The truncated potential is clearly adequate.

We also tested the convergence of the calculations towards truncation of the basis set in rotational quantum number j .

Table 4 summarizes the results for the partial wave $l = 6$ component of the total cross sections calculated for a total energy E of 1.0 eV from the three basis sets

TABLE 3
COMPARISON OF TOTAL CROSS SECTIONS FOR $E = 0.5$ eV
CORRESPONDING TO THE POTENTIALS (a) $V = v_0 + v_2P_2$
AND (b) $V = v_0 + v_2P_2 + v_4P_4 + v_6P_6$

$ \Delta j $	$j = j'$	σ (10^{-16} cm 2)	
		(a)	(b)
0.....	0 $\rightarrow$ 0	40.8	40.8
	2 $\rightarrow$ 2	41.1	41.1
	4 $\rightarrow$ 4	43.3	43.3
	6 $\rightarrow$ 6	45.4	45.4
2.....	0 $\rightarrow$ 2	4.01	4.11
	2 $\rightarrow$ 4	0.56	0.62
4.....	0 $\rightarrow$ 4	0.10	0.10
6.....	0 $\rightarrow$ 6	4.2×10^{-5}	3.8×10^{-5}

TABLE 4
PARTIAL CROSS SECTIONS FOR $l = 6$ CALCULATED
BY TRUNCATING THE BASIS SET AT
 $j_{\max} = 6, 8, \text{ AND } 10$ FOR $E = 1.0$ eV*

$j \rightarrow j'/j_{\max}$	6	8	10
0 $\rightarrow$ 0.....	0.194	0.194	0.194
2 $\rightarrow$ 2.....	0.094	0.094	0.094
4 $\rightarrow$ 4.....	0.336	0.334	0.334
6 $\rightarrow$ 6.....	0.609	0.569	0.568
0 $\rightarrow$ 2.....	0.119	0.119	0.119
2 $\rightarrow$ 4.....	0.052	0.051	0.051
0 $\rightarrow$ 4.....	0.020	0.020	0.020
0 $\rightarrow$ 6.....	0.001	0.001	0.001

* Cross sections are in 10^{-16} cm 2 .

in which the maximum j value retained was respectively 6, 8, and 10. Truncation of the basis set at $j = 6$ achieves convergence to within 3 percent.

V. TOTAL CROSS SECTIONS AND ANGULAR DISTRIBUTIONS

Calculations were carried out for total energies of 0.5, 1.0, and 1.5 eV. The potential was truncated at the v_2P_2 term, and the basis set of channels was truncated at $v = 0, j = 6$.

Figures 1 to 4 show the elastic differential cross sections ($d\sigma/d\Omega$) as a function of the scattering angle θ at $E = 0.5, 1.0, \text{ and } 1.5$ eV for the elastic processes

$$H + H_2(j) \rightarrow H + H_2(j), \quad j = 0, 2, 4, 6.$$

FIG. 1.—Differential cross sections ($d\sigma/d\Omega$) (in $\text{\AA}^2$) as a function of scattering angle θ (in degrees) for the elastic transition $H + H_2(j = 0) \rightarrow H + H_2(j' = 0)$. Curve A, $E = 0.5$ eV; B, $E = 1.0$ eV; C, $E = 1.5$ eV.

FIG. 2.—Differential cross sections ($d\sigma/d\Omega$) (in $\text{\AA}^2$) as a function of scattering angle θ (in degrees) for the elastic transition $\text{H} + \text{H}_2(j=2) \rightarrow \text{H} + \text{H}_2(j'=2)$. Curve A, $E = 0.5$ eV; B, $E = 1.0$ eV; C, $E = 1.5$ eV.

FIG. 3.—Differential cross sections ($d\sigma/d\Omega$) (in $\text{\AA}^2$) as a function of scattering angle θ (in degrees) for the elastic transition $\text{H} + \text{H}_2(j=4) \rightarrow \text{H} \pm \text{H}_2(j'=4)$. Curve A, $E = 0.5$ eV; B, $E = 1.0$ eV; C, $E = 1.5$ eV.

FIG. 4.—Differential cross sections ($d\sigma/d\Omega$) (in $\text{\AA}^2$) as a function of scattering angle θ (in degrees) for the elastic transition $\text{H} + \text{H}_2(j=6) \rightarrow \text{H} + \text{H}_2(j'=6)$. Curve A, $E = 0.5$ eV; B, $E = 1.0$ eV; C, $E = 1.5$ eV.

The cross sections $d\sigma/d\Omega(j \rightarrow j'|\theta)$ peak strongly in the forward direction, as is typical of heavy-particle scattering, the forward peak becoming more pronounced as the impact energy increases. This behavior occurs because scattering at small angles arises from larger values of l , and more partial waves contribute to the scattering as the impact energy increases.

FIG. 5.—Differential cross sections ($d\sigma/d\Omega$) (in $\text{\AA}^2$) as a function of scattering angle θ (in degrees) for the inelastic transition $\text{H} + \text{H}_2(j=6) \rightarrow \text{H} + \text{H}_2(j'=4)$ at $E = 0.5$ eV.

Figure 5 shows the angular dependence of the inelastic differential cross sections $d\sigma/d\Omega$ ($6 \rightarrow 4|\theta$). The inelastic differential cross sections are several orders of magnitude smaller than the elastic cross sections $Q(6-6|\theta)$, so that the inelastic angular distributions are of minor importance in astrophysical applications. Figure 5, however, exhibits an interesting feature of the inelastic scattering process. The cross section $d\sigma/d\Omega$ ($6 \rightarrow 4|\theta$) has a broad backward peak in addition to the forward peak. The backward peak shows that the inelastic scattering processes are sensitive to the repulsive anisotropy of the short-range part of potential, especially when the impact energy is high.

We present finally in Table 5 the cross sections for elastic scattering and for rotational transitions at total energies of 0.5, 1.0, and 1.5 eV.

TABLE 5
TOTAL CROSS SECTIONS FOR $H + H_2(j) \rightarrow H + H_2(j')$
AT $E = 0.5, 1.0$, AND 1.5 eV

$ \Delta j $	$j \rightarrow j'$	σ (10^{-16} cm ²)		
		$E = 0.5$	$E = 1.0$	$E = 1.5$
0.....	$0 \rightarrow 0$	41.2	38.7	37.1
	$2 \rightarrow 2$	41.3	38.6	36.7
	$4 \rightarrow 4$	43.4	40.4	38.3
	$6 \rightarrow 6$	45.4	42.6	40.4
2.....	$0 \rightarrow 2$	4.02	5.00	4.44
	$2 \rightarrow 0$	0.88	1.05	0.92
	$2 \rightarrow 4$	0.63	1.75	1.70
	$4 \rightarrow 2$	0.45	1.01	1.03
4.....	$4 \rightarrow 6$	0.014	0.48	0.83
	$6 \rightarrow 4$	0.018	0.43	0.63
	$0 \rightarrow 4$	0.104	0.437	0.344
	$4 \rightarrow 0$	0.017	0.055	0.043
6.....	$2 \rightarrow 6$	0.0004	0.046	0.068
	$6 \rightarrow 2$	0.0004	0.024	0.030
	$0 \rightarrow 6$	4.2×10^{-5}	0.007	0.008
	$6 \rightarrow 0$	8.5×10^{-6}	0.001	0.001

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