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Hyperspherical calculation for electron hydrogen atom ionization collisions in a symmetric form

J N DAS
Department of Applied Mathematics, University College of Science, 92, Acharya Prafulla Chandra Road, Calcutta 700 009, India
Email: jndas@cubmb.ernet.in

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Abstract. The hyperspherical partial wave method (Das [7]) has been presented here in a symmetric form so that effects of coupling among different partial waves may be included in a systematic way. It is also outlined here how to solve the relevant coupled set of radial wave equations numerically. Some preliminary results are presented for S, P and D waves in the low energy domain of 30–50 eV for the incident electron. In this calculation only two important partial waves are included in each channel. The results are compared with experimental ones and appear very encouraging.

Keywords. Hyperspherical; ionization; cross section; partial wave; channel; close-coupling.

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1. Introduction

Three very successful methods of calculating total cross sections for ionization of hydrogen atoms by electrons at low energies are the convergent close-coupling (CCC) method (Bray and Stelbovics [1, 2]), the R-matrix with pseudostates (RMPS) method (Bartschat *et al* [3]) and the hyperspherical close-coupling (HSCC) method (Kato and Watanabe [4]). All these methods give good total cross values (see [4, 5]) down to very low energies. However their capabilities in reproducing the differential cross sections have not been tested (except in one or two cases such as in Bray *et al* [6]). Moreover each of these methods has its own difficulties and limitations. Another, very similar approach, is the hyperspherical partial wave (HSPW) method, suggested by the present author [7]. This is perhaps a better approach. Since this approach is straightforward and most natural, it is just an extension of the partial wave method so useful in two-body scattering calculations. It is also free from any pathological difficulty such as the non-existence of certain integrals for some of the angular momenta for the partial waves (see the second paragraph after eq. (2) of ref. [6]). It also does not require additional knowledge such as in HSCC calculation where one needs the values of the wave function in the asymptotic domain for matching purpose from some other sources. Moreover such values are known only approximately and no analytic solution exists for the asymptotic domain. Some interesting results for differential cross sections at low energies have already been

obtained following this approach, for Erhardt asymmetric geometry [8] and for coplanar constant θ_{12} geometry [9], θ_{12} being the angle between the outgoing electrons. In these calculations effects of coupling among different partial waves, in hyperspherical coordinates, are neglected. To include the effects of coupling among different partial waves it will be better to proceed in a symmetric form as is indicated below. In our earlier papers [7–9] we did not consider the problem of how to solve the resultant coupled set of radial wave equations numerically. Here we paid attention to this very problem and outlined a method. Following the present approach some calculations have also been done. Here we report also these preliminary results. In § 3 we describe the present symmetric approach which intends to include fully the coupling effects. In § 3 we describe the calculations of the present article. Results for S, P and D waves are reported in § 4. Some concluding remarks are made in § 5.

2. Hyperspherical calculation in a symmetric form

We consider ionization of a hydrogen atom in its ground state by an electron of incidence energy E_i and momentum $\mathbf{p}_i$, the momentum of the ejected and scattered electrons being $\mathbf{p}_1$ and $\mathbf{p}_2$ and coordinates $\mathbf{r}_1$, $\mathbf{r}_2$.

Then ionization amplitude for symmetry S is given by

$$f^S = -(2\pi)^2 \langle \Psi_{fs}^{(-)} | V_i | \Phi_i \rangle, \tag{1}$$

where $S = 0$ or 1 corresponding to a symmetric or an antisymmetric wave function. Here

$$V_i(\mathbf{r}_1, \mathbf{r}_2) = (1/r_{12}) - (1/r_2),$$
$$\Phi_i(\mathbf{r}_1, \mathbf{r}_2) = (1/2\sqrt{2\pi^2}) e^{-r_1} \cdot e^{i\mathbf{p}_i \cdot \mathbf{r}_2}$$

and $\Psi_{fs}^{(-)}$ is the exact scattering state wave function in the final channel with symmetry S and satisfying incoming converging boundary condition. Here we indicate how one can calculate $\Psi_{fs}^{(-)}$, and hence the scattering amplitude using hyperspherical coordinates $(R, \alpha, \hat{r}_1, \hat{r}_2)$, where

$$R = \sqrt{r_1^2 + r_2^2}, \qquad \alpha = \tan^{-1}(r_2/r_1).$$

We set

$$P = \sqrt{p_1^2 + p_2^2}, \qquad \alpha_0 = \tan^{-1}(p_2/p_1)$$

and use the notations $\omega = (\alpha, \hat{r}_1, \hat{r}_2)$, $\omega_0 = (\alpha_0, \hat{p}_1, \hat{p}_2)$.

Now we note that plane wave has the expansion [7]

$$\exp(i\mathbf{p}_1 \cdot \mathbf{r}_1 + i\mathbf{p}_2 \cdot \mathbf{r}_2)/(2\pi)^3 = (2/\pi)^{1/2} \sum_\lambda i^\lambda (j_{\nu_\lambda}(\rho)/\rho^{3/2}) \varphi_\lambda^*(\omega_0) \varphi_\lambda(\omega), \tag{2}$$

where

$$\varphi_\lambda(\omega) = P_{l_1 l_2}^n(\alpha) Y_{l_1 l_2}^{LM}(\hat{r}_1, \hat{r}_2),$$

and $P_{l_1 l_2}^n$ is the Jacobi wave function and $Y_{l_1 l_2}^{LM}$ is the coupled angular momentum wave function. Here n, l_1, l_2, L are some non-negative integers and $-L \leq M \leq L$. L corresponds

to total angular momentum for the two electrons in the system and l_1, l_2 corresponds to angular momentum for the individual electrons.

Henceforth λ stands for the eigenvalue $l_1 + l_2 + 2n$ or the set (l_1, l_2, n, L, M) depending on the context and $\nu_\lambda = \lambda + 3/2$, $\rho = PR$. For our present formulation it is necessary to consider the symmetrized plane wave function, which may be expanded in hyperspherical coordinates using the symmetrized angular wave function [10]

$$\begin{aligned}\varphi_\lambda^S(\omega) &= (1/(2)^{1/2})\{P^n_{l_1 l_2}(\alpha)Y^{LM}_{l_1 l_2}(\hat{r}_1, \hat{r}_2) + (-1)^{l_1+l_2-L+S+n} \\ &\qquad \times P^n_{l_2 l_1}(\alpha)Y^{LM}_{l_2 l_1}(\hat{r}_1, \hat{r}_2)\} \quad \text{for } l_1 \neq l_2 \\ &= \tfrac{1}{2}[1 + (-1)^{-L+S+n}]P^n_{ll}(\alpha)Y^{LM}_{ll}(\hat{r}_1, \hat{r}_2), \quad \text{for } l_1 = l_2 = 1. \end{aligned} \tag{3}$$

These wave functions are orthonormal and have definite values of (L, M, S, π), π standing for parity and taking values 0 or 1. Then one can easily prove that

$$\begin{aligned}&\{\exp(i\mathbf{p}_1\cdot\mathbf{r}_1 + i\mathbf{p}_2\cdot\mathbf{r}_2) + (-1)^S \exp(i\mathbf{p}_1\cdot\mathbf{r}_2 + i\mathbf{p}_2\cdot\mathbf{r}_1)\}/(2\pi)^3 \\ &\quad = 2(2/\pi)^{1/2} \sum_{\substack{l_1 \le l_2 n \\ LM}} i^\lambda (j_{\nu_\lambda}(\rho)/\rho^{3/2})\varphi_\lambda^{S*}(\omega_0)\varphi_\lambda^S(\omega). \end{aligned} \tag{4}$$

We consider symmetrized final scattering state $\Psi_{\text{fs}}^{(-)}$ with incoming boundary condition. This state may be expanded as

$$\Psi_{\text{fs}}^{(-)}(R, \omega) = (2/\pi)^{1/2} \sum_{\substack{l_1 \le l_2 n \\ LM}} (F_\lambda^S(\rho)/\rho^{5/2})\varphi_\lambda^S(\omega). \tag{5}$$

The radial wave functions $F_\lambda^S(\rho)$'s satisfy the equations

$$[(\mathrm{d}^2/\mathrm{d}\rho^2) + 1 - (\nu_\lambda(\nu_\lambda + 1))/\rho^2]F_\lambda^S + \sum_{\lambda'} (2\gamma^S_{\lambda\lambda'}/\rho)F^S_{\lambda'} = 0, \tag{6}$$

where

$$\begin{aligned}&\gamma^S_{\lambda\lambda'} = (1/P)\langle\varphi_\lambda^S|C|\varphi_{\lambda'}^S\rangle, \\ &\quad C = (1/\cos\alpha) + (1/\sin\alpha) - (1/|\hat{r}_1\cos\alpha - \hat{r}_2\sin\alpha|). \end{aligned}$$

At this point an explanation is in order why the formulation of the problem in symmetric form is expedient. Because of conversation laws, for any fixed $\mu = (L, S, \pi)$ only radial waves with this particular μ enter in a coupled set of equations, reducing considerably the computational problem.

In the above equations those λ, λ' occur for which there are fixed values of L, M, S and π. For the present case $M = 0$ only needs consideration, since in the calculation of the scattering amplitude, given by equation (1), only states with $M = 0$ gives a non-zero contribution. Henceforth we fix $M = 0$ everywhere. Now we denote (L, S, π) by the single letter and introduce a single index N in place of (l_1, l_2, n). Then we have $F_\lambda^S(\rho) = f_N^\mu(\rho)$ and equation (6) becomes

$$[(\mathrm{d}^2/\mathrm{d}\rho^2) + 1 - ((\nu_N^\mu(\nu_N^\mu + 1)/\rho^2)]f_N^\mu(\rho) + \sum_{N'} (2\gamma^\mu_{NN'}/\rho)f^\mu_{N'}(\rho) = 0, \tag{7}$$

where $\nu_\lambda \equiv \nu_N^\mu$, $\gamma_{\lambda\lambda'}^S \equiv \gamma_{NN'}^\mu$ for each fixed μ and N. In any realistic calculation N, N' are restricted to certain maximum value $N_{mx} \cdot N_{mx}$ depends on μ, but this will not be explicitly indicated here.

Now we consider particular solutions of the above set of equations. It may be noted that there are two particular sets of solutions $\mathbf{f}_{sn}^{\mu(k)}(\rho)$ and $\mathbf{f}_{cs}^{\mu(k)}(\rho)$ which behave asymptotically as

$$f_{snN}^{\mu(k)}(\rho) \sim a_{kN}^\mu \sin(\rho + \beta_k^\mu \ln 2\rho), \quad \rho \to \infty$$

and

$$f_{csN}^{\mu(k)}(\rho) \sim b_{kN}^\mu \cos(\rho + \beta_k^\mu \ln 2\rho), \quad \rho \to \infty.$$

Here β_k^μ is the kth eigenvalue of the charge matrix $A^\mu = (\gamma_{NN'}^\mu)$ and

$$\mathbf{X}_k^\mu = \begin{pmatrix} a_{k1}^\mu \\ \vdots \\ a_{kN_{mx}}^\mu \end{pmatrix}, \qquad \mathbf{Y}_k^\mu = \begin{pmatrix} b_{k1}^\mu \\ \vdots \\ b_{kN_{mx}}^\mu \end{pmatrix}$$

are the kth eigenvectors of it. We determine particular solutions $\mathbf{f}_{sn}^{\mu(k)}$ and $\mathbf{f}_{cs}^{\mu(k)}$ in the asymptotic region by substituting

$$f_N(\rho)^{\mu(k)} = \sum_{l=0}^{\infty} a_{kN}^{\mu(l)} (\sin\theta_k^\mu / \rho^l) + \sum_{l=0}^{\infty} b_{kN}^{\mu(l)} (\cos\theta_k^\mu / \rho^l), \tag{8}$$

where $\theta_k^\mu = \rho + \beta_k^\mu \ln 2\rho$ in the differential equation (7) and on equating coefficients of $\sin\theta_k/\rho^{l+1}$ and $\cos\theta_k/\rho^{l+1}$ to zero. Thus we have the following recurrence relations for the unknowns

$$\begin{aligned} 2[(A_k^\mu)^2 + l^2]X_k^{\mu(l)} &= [A_k^\mu \Lambda_k^\mu - l(l-1)A_k^\mu - l(2l-1)\beta_k^\mu I]\mathbf{X}_k^{\mu(l-1)} \\ &\quad - [(2l-1)\beta_k^\mu A_k^\mu + l\Lambda_k^\mu - l^2(l-1)I]\mathbf{Y}_k^{\mu(l-1)}, \qquad (9a) \\ 2[(A_k^\mu)^2 + l^2]\mathbf{Y}_k^{\mu(l)} &= [A_k^\mu \Lambda_k^\mu - l(l-1)A_k^\mu - l(2l-1)\beta_k^\mu I]\mathbf{Y}_k^{\mu(l-1)} \\ &\quad + [(2l-1)\beta_k^\mu A_k^\mu + l\Lambda_k^\mu - l^2(l-1)I]\mathbf{X}_k^{\mu(l-1)}, \qquad (9b) \end{aligned}$$

where

$$\begin{aligned} &(\mathbf{X}_k^{\mu(l)})_N = a_{kN}^{\mu(l)}, \quad (\mathbf{Y}_k^{\mu(l)})_N = b_{kN}^{\mu(l)}, \\ &A_k^\mu = A^\mu - \beta_k^\mu I, \quad (\Lambda_k^\mu)_{NN'} = [(\beta_k^\mu)^2 + \nu_N^\mu(\nu_N^\mu + 1)]\delta_{NN'}. \end{aligned}$$

The above equations with the initial conditions

$$\mathbf{X}_k^{\mu(0)} = \mathbf{X}_k^\mu, \quad \mathbf{Y}_k^{\mu(0)} = \mathbf{0}$$

give $\mathbf{f}_{sn}^{\mu(k)}(\rho)$ and the conditions

$$\mathbf{X}_k^{\mu(0)} = \mathbf{0}, \quad \mathbf{Y}_k^{\mu(0)} = \mathbf{X}_k^\mu$$

give $\mathbf{f}_{cs}^{\mu(k)}(\rho)$. The functions $f_{snN}^{\mu(k)}(\rho)$'s and $f_{csN}^{\mu(k)}(\rho)$'s are then continued from asymptotic region downwards by numerical integration of the differential equation (7).

Now the physical solution will be a superposition

$$f_N^{\mu}(\rho) = \sum_k c_k^{\mu} f_{snN}^{\mu(k)}(\rho) + \sum_k d_k^{\mu} f_{csN}^{\mu(k)}(\rho). \tag{10}$$

The partial wave containing $\varphi_{\lambda_N}^S(\omega)$ will be then

$$(2/\pi)^{1/2} \sum_k (c_k^{\mu} + id_k^{\mu}) a_{kN}^{\mu} (\exp(i(\rho + \beta_k^{\mu} \ln 2\rho))/2i\rho^{5/2}) \varphi_{\lambda_N}^S(\omega),$$

λ_N corresponds to the set λ for the index N and for fixed μ. This must agree (apart from a Coulomb distortion) with the part

$$2(2/\pi)^{1/2} i^{\lambda_N} \exp(i(\rho - \nu_N^S \pi/2))/2i\rho^{5/2}) \varphi_{\lambda_N}^{S*}(\omega_0) \varphi_{\lambda_N}^S(\omega)$$

of the symmetrized plane wave in order that $\Psi_{\text{fs}}^{(-)}$ be asymptotically a superposition of (distorted) symmetrized plane wave plus incoming converging waves. So we have,

$$\sum_k (c_k^{\mu} + id_k^{\mu}) a_{kN}^{\mu} = 2\exp(i(\lambda_n - \nu_N)\pi/2) \varphi_{\lambda_N}^{S*}(\omega_0). \tag{11}$$

Putting $p_k^{\mu} = c_k^{\mu} + id_{k'}^{\mu}$, $q_k^{\mu} = c_k^{\mu} - id_k^{\mu}$ we have

$$X^{\mu}\mathbf{P}^{\mu} = -2\exp(i\pi/4) \begin{pmatrix} \varphi_1^{\mu*}(\omega_0) \\ \vdots \\ \varphi_{Nmx}^{\mu*}(\omega_0) \end{pmatrix},$$

where

$$\mathbf{P}^{\mu} = \begin{pmatrix} p_1^{\mu} \\ \vdots \\ p_{N_{mx}}^{\mu} \end{pmatrix} \quad \text{and } X^{\mu} = (\mathbf{X}_1^{\mu}, \mathbf{X}_2^{\mu}, \ldots, \mathbf{X}_{N_{mx}}^{\mu}).$$

Then

$$\mathbf{P}^{\mu} = -2\exp(i\pi/4)(X^{\mu})^{-1} \begin{pmatrix} \varphi_1^{\mu*}(\omega_0) \\ \vdots \\ \varphi_{N_{mx}}^{\mu*}(\omega_0) \end{pmatrix}. \tag{12}$$

Here the inverse $(X^{\mu})^{-1}$ exists since X^{μ} is actually the similarity transformation which diagonalizes the symmetric charge matrix A^{μ}.

Next we construct N_{mx} independent solutions of equation (7) which vanish at origin. We denote the corresponding solution vectors by $\mathbf{f}_0^{\mu(k)}$, $k = 1, 2, \ldots, N_{mx}$. Then the physical solution vector may also be written as

$$\mathbf{f}^{\mu}(\rho) = \sum_k \frac{1}{2} G_k \mathbf{f}_0^{\mu(k)}(\rho). \tag{13}$$

We match values of radial waves (and their derivatives) given by right hand sides of equations (10) and (13) at some $\rho = \rho_{\text{int}}$. This gives remaining unknown constants $q_k^{\mu} = c_k^{\mu} - id_k^{\mu}$ in (10). Thus finally we have the physical solutions in the above forms. In

particular we have

$$f_N^{\mu}(\rho) = \frac{1}{2}\sum_k (g_{RK} + ig_{IK}) f_{0N}^{\mu(k)}(\rho), \tag{14}$$

where g_{RK} and g_{IK} turns out in the forms

$$g_{RK} = \sum_{N'} g_{KN'}^{(1)} \varphi_{N'R}^{\mu}(\omega_0) + \sum_{N'} g_{KN'}^{(2)} \varphi_{N'I}^{\mu}(\omega_0)$$

and

$$g_{IK} = \sum_{N'} g_{KN'}^{(3)} \varphi_{N'R}^{\mu}(\omega_0) + \sum_{N'} g_{KN'}^{(4)} \varphi_{N'I}^{\mu}(\omega_0), \tag{15}$$

and $\varphi_{N'R}^{\mu}(\omega_0)$ and $\varphi_{N'I}^{\mu}(\omega_0)$ are the real and imaginary parts of $\varphi_{N'}^{\mu}(\omega_0)$. In this way radial waves $f_N^{\mu}(\rho)$'s are determined for the scattering states

$$\Psi_{\mathrm{fs}}^{(-)}(\rho) = (2/\pi)^{1/2} \sum_{\lambda_N} (f_N^{\mu}(\rho)/\rho^{5/2}) \varphi_{\lambda_N}^{S}(\omega). \tag{16}$$

This on substituting in equation (1) gives the scattering amplitude and hence the cross sections.

3. Calculations

From the results of CCC and RMPS calculations of Bartschat and Bray [5] it is now known that at low energies S, P and D waves give most significant contributions to the total cross section, P wave itself accounting for more than 50%. So we include in our calculations only the channel $^{1,3}S^e$, $^{1,3}P^0$ and $^{1,3}D^e$. Here a channel corresponds to fixed values of $(L, S, P) = \mu$. We report two sets of results. In one of these only one, most important, partial wave in each channel is retained. For example $^3P^0$ includes the partial wave with $l_1 = 0, l_2 = 1, n = 0$ only. In the second calculation we include two important partial waves in each channel. These are shown in table 1.

In our present scheme, determination of solution of the coupled set of equations [7] is the most difficult task. As is described in §2 the equations are solved by matching method. In the asymptotic domain solutions $\mathbf{f}_{sn}^{(k)}(\rho)$ and $\mathbf{f}_{cs}^{(k)}(\rho)$ are determined from asymptotic expansion (equations (8) and (9)). Then another set of solutions are continued from the neighbourhood of origin, say starting at ε (with $\varepsilon = 0.1$). At this point N_{mx} solutions are constructed with initial values zero and derivatives δ_{NK} for the Nth element of the kth solution vector. These are then continued numerically to ρ_{int}, a point in the asymptotic domain. In this numerical integration of the equations (8) we adopted a Tailors expansion with 10 terms in steps $\Delta\rho = 0.01$ initially up to 0.2, then in steps $\Delta\rho = 0.05$ up to 0.2, then with $\Delta\rho = 0.2$ up to ρ_∞, a point beyond which no contribution arises in the T-matrix elements. ρ_{int} was varied from 20 a.u. to about 150 a.u. in steps of 5 or 10 a.u.. In general there was good agreement in the results for different matching points ρ_{int}. But occasionally there were oscillations also. In some instances there were some spurious singular like behaviours. With further change in the value of ρ_{int}, the results again become what it should be. The results presented in the next section were obtained from observation of

Table 1. First two important partial waves with parameters (l_1, l_2, n) included in different channels in the present calculations.

$^1S^e$	$^3S^e$	$^1P^0$	$^3P^0$	$^1D^e$	$^3D^e$
(0,0,0)	(0,0,1)	(0,1,0)	(0,1,0)	(1,1,0)	(1,1,1)
(0,0,2)	(0,0,3)	(0,1,1)	(0,1,1)	(1,1,2)	(1,1,3)

Table 2. Partial wave cross sections (in a_0^2) for ionization of hydrogen atoms by electrons in different channels in the energy range 30–50 eV for calculations with $N_{mx} = 2$. Quantities in brackets represent those with $N_{mx} = 1$. Total cross sections are also presented (which include cross section for F state of RMPS calculations). See text for details.

E_i (eV)	$\sigma(^1S^e)$	$\sigma(^3S^e)$	$\sigma(^1P^0)$	$\sigma(^3P^0)$	$\sigma(^1D^e)$	$\sigma(^3D^e)$	σ_{Tot}	σ_{Tot} (CCC)	σ_{Tot} (RMPS)
30	0.08	0.02	0.06	0.32	0.12	0.00	0.63	0.60	0.58
	(0.06)	(0.00)	(0.02)	(0.36)	(0.19)	(0.02)			
35	0.10	0.03	0.06	0.28	0.13	0.01	0.65	0.65	0.63
	(0.05)	(0.00)	(0.01)	(0.26)	(0.17)	(0.02)			
40	0.08	0.05	0.07	0.27	0.12	0.01	0.64	0.68	0.66
	(0.04)	(0.00)	(0.01)	(0.19)	(0.14)	(0.01)			
45	0.06	0.05	0.08	0.25	0.11	0.01	0.59	0.70	0.68
	(–)	(–)	(–)	(–)	(–)	(–)			
50	0.06	0.03	0.07	0.24	0.09	0.01	0.53	0.71	0.69
	(–)	(–)	(–)	(–)	(–)	(–)			

results calculated with different ρ_{int} in the range noted above. Often average values were taken as the final results. In these calculations scaling of the wave functions is necessary, since for a variation of ρ from say $\rho = 1.0$ to $\rho = 10$ units the wave function changes by many orders. As already stated we made calculations for $N_{mx} = 1$ and $N_{mx} = 2$ only. For further increase of N_{mx} often the results become unphysical. This implies that then stabilization of the calculations becomes essential. This problem is left for a future investigation. Now in obtaining T-matrix elements all the integrations except the integration over ρ were done analytically. The ρ-integration was done numerically. In calculating the partial cross sections from the T-matrix elements the remaining integrations are amenable to analytical evaluations. In this paper we present only the various partial cross sections and values of certain parameters related to these.

4. Results

Partial wave cross sections for ionization of hydrogen atoms by electrons in the energy range 30–50 eV of our present calculation are presented in table 2. In this table two sets of results are presented. One set corresponds to $N_{mx} = 2$ and for comparison a second set is presented for $N_{mx} = 1$. For 30, 35 and 40 eV energies the two sets of results are close to each other indicating that at these energies most important contributions arises from single states (0,0,0) in $^1S^e$, (0,0,1) in $^3S^e$, (0,1,0) in $^1P^0$ and $^3P^0$, (1,1,0) in $^1D^e$ and (1,1,1) in $^3D^e$. As the energy increases, other states in these channels become important. The two

Table 3. Ratio of partial wave cross section to total cross section for ionization of hydrogen atoms by electrons for different total angular momentum L.

L	$E_i = 30\,eV$			$E_i = 50\,eV$		
	Present ($N_{mx} = 2$)	RMPS	CCC	Present ($N_{mx} = 2$)	RMPS	CCC
0	0.14	0.10	0.13	0.16	0.09	0.09
1	0.63	0.63	0.51	0.57	0.60	0.56
2	0.20	0.23	0.28	0.17	0.24	0.26
3	–	0.05	0.10	–	0.06	0.09

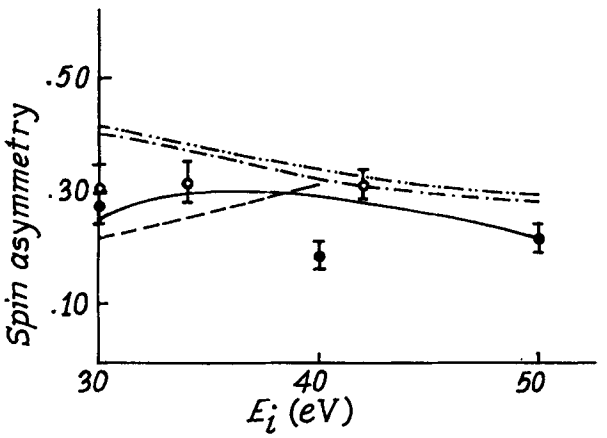

Figure 1. Spin asymmetry for electron impact ionization of hydrogen atoms as a function of the projectile energy. Theory: continuous, present calculation; dash-dotted, CCC [5]; dash-double dotted, RMPS [5]. Experiment: •, Crowe *et al* [12]; ○, Fletcher *et al* [11].

states shown in table 1 in each channel give reasonable contributions to partial cross sections as well as to total cross sections in the energy range 30–40 eV. Total cross sections of the present calculation, the CCC and the RMPS calculations agree quite well (see table 2). Beyond 40 eV, however, the results go to depart considerably. We have not calculated F-channel contributions. F-channel gives about 5% to 10% contributions to the total cross sections at these energies. In calculating the total cross sections we have included the F-channel values of RMPS calculation to our results. Next we look to table 3 where we presented ratios of partial cross sections to the total cross sections. Our results agree well with the CCC results and with the RMPS results for 30 eV energy. For 50 eV energy our S-wave results appear somewhat higher compared to those of other calculations, while the D-wave cross sections are somewhat lower. The P-wave cross sections of these calculations which account for more than 50%, agree reasonably well with one another.

Finally in figure 1 we have presented values of an important parameter of these cross section results. This is the spin asymmetry parameter defined by

$$\text{spin asymmetry} = (\sigma^S - \sigma^T)/(\sigma^S + 3\sigma^T).$$

We have compared our computed values of this parameter with those of CCC and RMPS calculations and with the experimental results of Fletcher *et al* [11] and Crowe *et al* [12]. It is interesting to note that our results for $N_{mx} = 2$ agree beautifully with the experimental results and appear somewhat better compared to the CCC and RMPS results in the above energy range. Excepting one point of Crowe *et al* all these experimental points are very close to our theoretical curve.

5. Conclusion

The results of our present preliminary calculation of electron hydrogen atom ionization collisions, presented here in a symmetric form, and which includes fully the coupling effects, appear very encouraging. Thus simple inclusion of two most important states in each channel gives good representation of the partial wave cross sections in the energy range 30–40 eV. However, for better results and for other energies, one has to include larger number of states in each channel. Matching method also does not appear very efficient. Improved calculations including a large number of partial waves in each channel now appears relatively difficult. Then stabilization of the calculation for the solution of the coupled set of equations will be necessary. Once this is achieved many interesting results and insights in the low energy domain are expected.

References

[1] I Bray and A Stelbovics, *Phys. Rev. Lett.* **69**, 53 (1992)
[2] I Bray and A Stelbovics, *Phys. Rev.* **A46**, 6995 (1992)
[3] K Bartschat, E T Hudson, M P Scott, P G Burke and V M Burke, *J. Phys.* **B29**, 115 (1996)
[4] D Kato and S Watanabe, *Phys. Rev. Lett.* **74**, 2443 (1995)
[5] K Bartschat and I Bray, *J. Phys.* **B29**, L577 (1996)
[6] I Bray, D A Konovalov, I E McCarthy and A T Stelbovics, *Phys. Rev.* **A50**, R2818 (1994)
[7] J N Das, *Aust. J. Phys.* **47**, 743 (1994)
[8] J N Das and K Chakrabarti, *Parmana – J. Phys.* **47**, 249 (1996)
[9] J N Das and K Chakrabarti, *Phys. Rev.* **A56**, 365 (1997)
[10] C D Lin, *Phys. Rev.* **A10**, 1986 (1974)
[11] G D Fletcher, M J Alguard, T J Gray, P F Wainwright, M S Lubell, W Raith and V W Hughes, *Phys. Rev.* **A31**, 2854 (1985)
[12] D M Crowe, X Q Guo, M S Lubell, J Slevin and M Eminyan, *J. Phys.* **B23**, L325 (1990)