Double differential cross sections for ionization of hydrogen atoms by electron impact in hyperspherical partial wave theory

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Abstract

The calculated double differential cross sections for 60eV energy, where the cross sections are also maximum, agree with the measure results of Shyn (1992) in a much better way compared to other theories for such energies.

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With the availability of results of some recent calculations of Bray (2002) and Röder et al (2003) and Das et al (2003a,b) the status of theoretical studies has reached a new epoch. Even then much remains to be done. For example, although the convergent close coupling (CCC) approach (Bray, 2000) gives beautiful the total, single, and the triple differential cross sections (for some kinematic conditions), it miserably fails in reproducing the double differential cross sections (DDCS) for intermediate and high energies. As regards the DDCS results the same is true for 3C theory (Berakdar and Klar, 1993). Results of external complex scaling (ECS) approach, now a famous approach, are not available, possibly due to difficulties. In this letter we present DDCS results of a calculation in hyperspherical partial wave approach (HPW) for 60eV energy, a typical intermediate energy, for which the cross sections are known to have maximum values.

The hyperspherical partial wave approach has been described in detail in (Das et al, 2003a) and also in greater detail in (Das, 1998). In this approach the scattering state wave function is expanded in symmetrized hyperspherical harmonics (Das, 1998; Das et al, 2003a) resulting in sets of infinite coupled equations in infinite number of radial wave functions in hyper radius $R$. After truncating these equations to some finite $N_{mx}^L$ numbers keeping the same number of radial wave functions one has to solve these over the semi-infinite interval $(0, \infty)$. In this calculation we have chosen $N_{mx}^L=40$ for $L=0$ and 1 and $N_{mx}^L=80$ for other $L$ values. Here $L$ values up to 12 has been found to be practically sufficient. For convenience in solution of the equations over $(0, \infty)$ we divide it into three subintervals $(0, \Delta)$, $(\Delta, R_\infty)$, $(R_\infty, \infty)$. As usual we have chosen $\Delta$, 5.0 a.u.. The asymptotic range parameter $R_\infty$ has to be properly chosen. We have set our codes in such a way that this parameter $R_\infty$ may be made to take values thousands of atomic units. This is possible only for another approach, the hyperspherical R-matrix method with semi classical outgoing waves (HRM-SOW) approach of Malegat et al (2000). Now inclusion of a large number of $L$ values, at the same time makes the calculation very time consuming. So with our moderate resources we have included values of $L$ up to 12 and chosen $R_\infty$ about 300 a.u.. With this choice we have moderately converged results.

In our present calculation our main interest is in the DDCS results. However we have also calculated single and total ionization cross sections to have a complete picture. The single differential cross sections have approximately converged except at the two ends, where energy of one of the electrons is below 2eV and where contamination with high Rydberg states gives unacceptable very high cross section results as in ECS calculation by Flux method (Baertschy et al 2001).

In figure 1 we have presented the calculated SDCS results, fourth order parabolic fitted cross section curves (singlet, triplet and total) have also been included. From these fitted SDCS results total cross sections (singlet, triplet and their sum) have also been calculated, as also the asymmetry parameter $A$. These results have been presented in table 1. Finally in figure 2 we have presented the DDCS results which is our main
objective, here DDCS results have been normalized in a way that the integrated single
differential cross sections agree with the parabolic fitted values. The results beautifully
agree with the measured results for energies below 6eV of the ejected electron. Particu-
larly the agreement with experiment for 3eV and 4eV are remarkable (see fig.2). Here the
normalization factors are also very close to unity. No earlier calculation could produce
such accurate results (see for example figures 8 and 12 of Bray (2000) and figures 5-7
of Berakdar and Klar (1993) for some other intermediate values. Unfortunately their
results for this particular energy of 60eV are not available.

In conclusion it may be said that the hyperspherical partial wave theory is successful
in reproducing the DDCS results, generally, in a far better manner compared to other
theories. If we recall its capability in describing ionization events from close to threshold
(viz. 1eV, 0.5eV and 0.3eV excess energies as in Das et al 2003b) to a few Rydberg
energy (Das 2002; Das et al 2003a) and the present one then the hyperspherical partial
wave theory may be claimed to have an edge over other theories. With the availability of
better computational facilities this claimed may be better established. More experi-
mental results, both double and triple differential cross sections, for intermediate energies
are urgently needed for better assessment of different sophisticated theories.

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Figure Captions

**Figure 1.** Single differential cross sections of the present calculation as compared with the experimental results of Shyn (1992).

**Figure 2.** Double differential cross sections of the present calculation as compared with the experimental results of Shyn (1992). The results have been normalized by factors, indicated in the figures, for the integrated single differential cross section to agree with the parabolic fitted results of figure 1.
Table

Table 1. Singlet, triplet and the total ionization cross section (in $10^{-8}$ cm) together with the spin asymmetry parameter $A$ of the present calculation at 60 eV energy as compared with the experimental results. Starred results correspond to the energy indicated in the bracket.

|       | $\sigma_0$ | $\sigma_1$ | $\sigma_T$ | $A$ |
|-------|------------|------------|------------|-----|
| Present| 35.7       | 53.5       | 89.2       | 0.200 |
| Experiment |           |            |            |     |
| Shyn:    | -          | -          | 87.0       | -   |
| Fite and Brackmann: | -          | -          | 72.0       | -   |
| Shah et al: | -          | -          | 51.3       | -   |
| Fletcher et al: | -          | -          | -          | 0.236* ± 0.021 (57 eV) |

$\sigma_0$, $\sigma_1$, and $\sigma_T$ are the singlet, triplet, and total ionization cross sections, respectively, in $10^{-8}$ cm. $A$ is the spin asymmetry parameter.
Figure 1
Figure 2