PRAMANA © Indian Academy of Sciences Vol. 53, No. 5
— journal of November 1999
physics pp. 869–875

Energy spectrum of ejected electrons in ionization of hydrogen atoms by electrons

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

MS received 19 May 1998; revised 18 June 1999

Abstract. Energy spectrum of ejected electrons in ionization of hydrogen atoms has been calculated following a multiple scattering theory of Das and Seal [15]. The results show peaks around two to three Rydbergs of energies of the ejected electrons, for incident electron energy of 250 eV and 500 eV, considered here, and for different combinations of the angular variables of the scattered and the ejected electrons, for scattering in a plane. The peaks are very similar to those observed in relativistic K-shell ionization of Ag atoms by electrons at 500 KeV energy [6]. The physical origin of these peaks may be traced to the second order scatterings, scattering first by the atomic nucleus (or the atomic electron) and then a second time by the atomic electron. These peaks are, however, absent in the first Born results. Experimental verification of the present results and theoretical calculation by some other well-known methods will be interesting.

Keywords. Cross-section; collision; ionization; spectrum; electron.

PACS No. 34.80 Dp

1. Introduction

The triply differential cross-section (TDCS) study in electron hydrogen atom ionization collisions has become increasingly interesting over the last two decades both theoretically and experimentally for relativistic [1–8] as well as for non-relativistic energies [9–15]. Capabilities of different theoretical models in reproducing various features of experimental results have been widely tested for different kinematical conditions. Cases for Ehrhardt kinematical conditions have been most extensively studied, for different energies of the incident electrons – from very low to high energies. One may refer for example, to the works of Brauner, Briggs and Klar [BBK] and of Das and Seal [15]. BBK theory however, gives qualitatively good results, but quantitatively not that good, particularly for low energies. Theory of Das and Seal often gives better quantitative results. Study of energy spectrum of ejected electrons could be very interesting. To our knowledge there is no such study, theoretical or experimental, reported in the literature, in the non-relativistic domain. There is, however, integrated cross-section results [14], which do not show much interesting features. The energy spectrum of ejected electrons in ionization of Ag atoms by relativistic electrons, as experimentally investigated by Schüle and Nakel [6] and theoretically calculated by Das and Dhar [16] open up the possibilities of investigating the corresponding problem for light atoms, like hydrogen and helium, for non-relativistic energies. Here we made such a calculation for hydrogen atmos for 250 eV and 500 eV energies of the incident electrons for various combinations of the scattering and ejection angles for scattering in a plane. In this calculation the multiple scattering theory of Das and Seal [15] has been used. The results do exhibit very interesting features. There are peaks at about two to three Rydbergs of energy. A detailed study reveals that these peaks are due to second order scatterings, first by atomic nucleus (or atomic electron) and then a second time by the atomic active electron. Such peaks are absent in first Born results and these need experimental verifications. It may be noted that the multiple scattering theory of Das and Seal [15] proved very successful in the study of TDCS results (see [15] and also [16]).

2. Theory

The direct T-matrix element for ionization of hydrogen atoms by electrons, may be written, following Das and Seal [14], as

$$T_{fi} = \langle \Phi_f^{(-)}(\mathbf{r}_1,\mathbf{r}_2)|V_i(\mathbf{r}_1,\mathbf{r}_2)|\Phi_i(\mathbf{r}_1,\mathbf{r}_2)\rangle. \tag{1}$$

Here $\mathbf{r}_1,\mathbf{r}_2$ represent the coordinates of the atomic active electron and the incident electron. $(\mathbf{p}_1,\mathbf{p}_2)$ and (E_1,E_2) represent the momenta and energies of the two electrons in the final state and $(\mathbf{p}_i,E_i)$ are the momentum and the energy of the incident electron. In eq. (1) we have the wave functions

$$\Phi_i(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{2\sqrt{2}\pi^2}\mathrm{e}^{-r_1}\ \mathrm{e}^{i\mathbf{p}_i\cdot\mathbf{r}_2} \tag{2a}$$

and

$$\begin{aligned}\Phi_f^{(-)}(\mathbf{r}_1,\mathbf{r}_2) = N\{&\varphi_{\mathbf{p}_1}^{(-)}(\mathbf{r}_1)\mathrm{e}^{i\mathbf{p}_2\cdot\mathbf{r}_2} + \varphi_{\mathbf{p}_2}^{(-)}(\mathbf{r}_2)\mathrm{e}^{i\mathbf{p}_1\cdot\mathbf{r}_1}\\ &+\varphi_{\mathbf{p}}^{(-)}(\mathbf{r})\mathrm{e}^{i\mathbf{P}\cdot\mathbf{R}} - 2\mathrm{e}^{i\mathbf{p}_1\cdot\mathbf{r}_1+i\mathbf{p}_2\cdot\mathbf{r}_2}\}/(2\pi)^3,\end{aligned} \tag{2b}$$

where

$$\begin{aligned}\mathbf{r} &= (\mathbf{r}_2-\mathbf{r}_1)/2, \qquad &\mathbf{R} &= (\mathbf{r}_2+\mathbf{r}_1)/2\\ \mathbf{p} &= (\mathbf{p}_2-\mathbf{p}_1), \qquad &\mathbf{P} &= (\mathbf{p}_2+\mathbf{p}_1)\end{aligned} \tag{2c}$$

and $\varphi_q^{(-)}(\mathbf{r})$ is the Coulomb wave function given by

$$\varphi_{\mathbf{q}}^{(-)}(\mathbf{r}) = \mathrm{e}^{\pi\alpha/2}\Gamma(1+i\alpha)\mathrm{e}_1^{i\mathbf{q}\cdot\mathbf{r}}F_1(-i\alpha,1,-i(qr+\mathbf{q}\cdot\mathbf{r})) \tag{2d}$$

with

$$\begin{aligned}&\alpha = 1/p_1,\ \text{ for }\ \mathbf{q}=\mathbf{p}_1;\ \ \alpha = 1/\mathbf{p}_2,\ \text{ for }\ \mathbf{q}=\mathbf{P}_2;\\ &\text{and }\ \alpha=-1/p,\ \text{ for }\ \mathbf{q}=\mathbf{p}\end{aligned} \tag{2e}$$

and N is a normalization constant given in Das and Seal [15].

The perturbation potential V_i is given by

$$V_i(\mathbf{r}_1, \mathbf{r}_2) = \left(\frac{1}{\mathbf{r}_{12}} - \frac{1}{\mathbf{r}_2}\right). \tag{3}$$

The direct T-matrix element is then given by

$$f(\mathbf{p}_1, \mathbf{p}_2) = -(2\pi)^2 T_{fi}, \tag{4a}$$

and the exchange amplitude by

$$g(\mathbf{p}_1, \mathbf{p}_2) = f(\mathbf{p}_2, \mathbf{p}_1). \tag{4b}$$

The triply differential cross-section is finally given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega_1 \mathrm{d}\Omega_2 \mathrm{d}E_1} = \frac{p_1 p_2}{p_i}\left[\frac{3}{4}|\mathbf{f} - \mathbf{g}|^2 + \frac{1}{4}|\mathbf{f} + \mathbf{g}|^2\right]. \tag{5}$$

3. Results and discussion

Results of our calculation are presented in figures 1a–f for 250 eV incident electron energy and in figures 2a–d for 500 eV incident electron energy. Cross-sections curves are presented against energy E_1 of the ejected electron in the range 5 eV–100 eV for different combinations of the angles of the scattered and the ejected electrons, scattering taking place in a plane. Cross-section results for first Born calculation are also presented in these curves. Let us now discuss about some important features of these results. Let us first look at figure 1a which represents results for $E_i = 250$ eV, $\theta_2 = -5°$ and $\theta_1 = 40°$. Here first Born results appear to be very large compared to the results of the present calculation for $E_1 < 20$ eV. The present results show a large peak at about 40 eV. In contrast to this the first Born result falls off very smoothly with the increase of energy. For $\theta_1 = 80°$ and other parameters remaining same as above, the cross-section curves, given in figures 1b, are more or less similar, except that the peak positions get shifted to lower energies. For $\theta_2 = -10°$, the cross-section curves given in figures 1c, d are somewhat different, compared to those given in figures 1a, b. The peaks are shifted to still lower energies (at about 25 eV). Here again for lower values of E_1 the first Born results and the results of the present calculation differ drastically. But with the increase in the value of E_1, the two sets of results go to coincide particularly for $\theta_1 = 80°$. For θ_2 still large in magnitude, as in case of $-20°$, the cross-section curves of the present calculation show much undulations. For $\theta_2 = -20°$ and $\theta_1 = 40°$ the results show a very sharp peak. In these cases the results of the first Born calculation are very different (see figures 1e, f). Next we look to figures 2a–d, which show results for 500 eV energy for the incident electron. Here also the first Born results differ considerably from those of the present calculation. For $\theta_2 = -5°$, the nature of the curves are similar to those for 250 eV incident electron energy (compare figures 2a, b with those of 1a, b). Only the peak positions get shifted to lower energies. For $\theta_2 = -10°$, $\theta_1 = 40°$ (figure 2c) and $\theta_1 = 80°$ (figure 2d), the cross-section curves are again more or less similar to those for 250 eV energy.

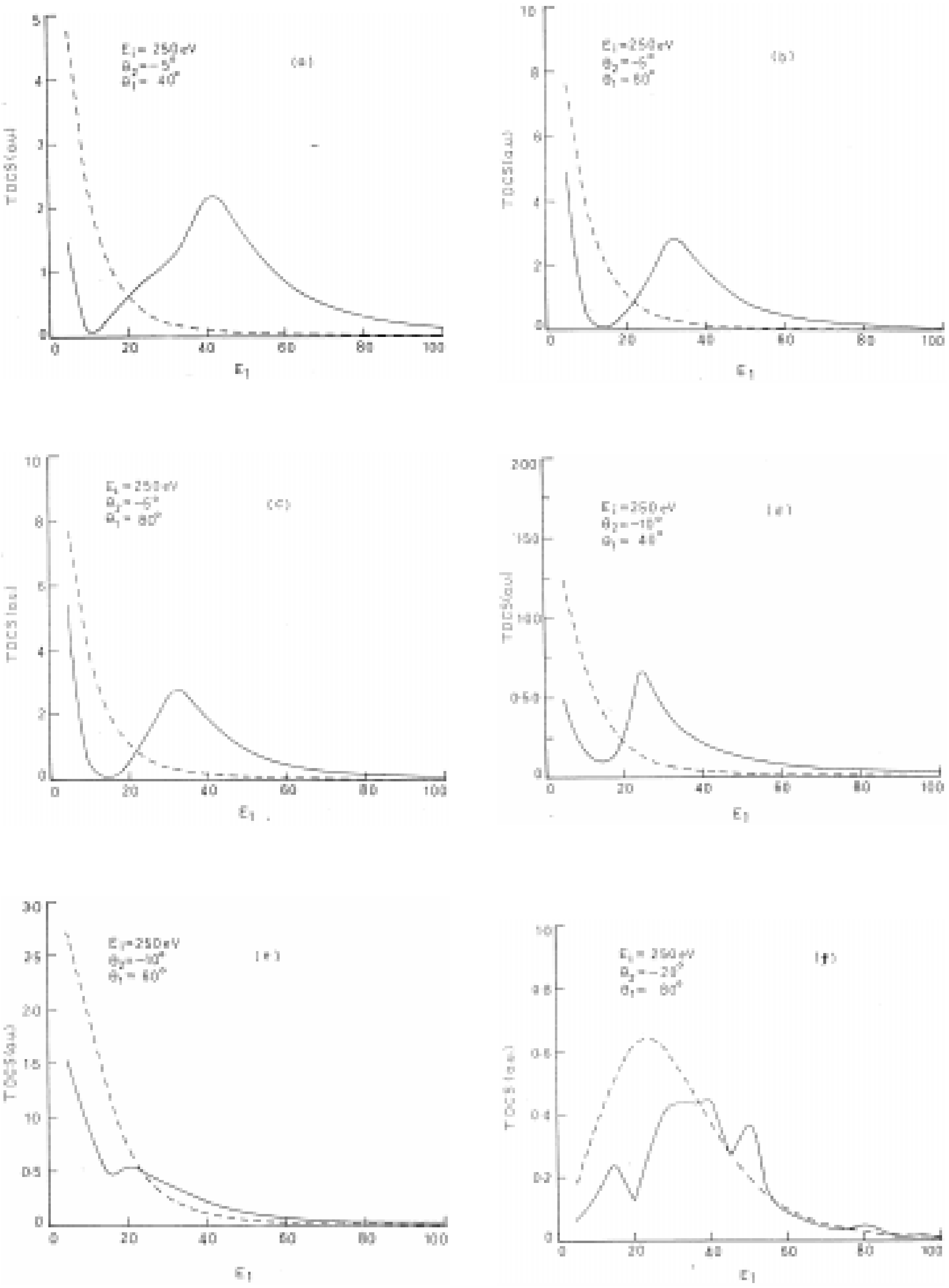

Figure 1a–f. Triply differential cross sections for ionization of hydrogen atoms by electrons shown against ejected electron energy E_1 for 250 eV incident electron energy E_i for different combinations of scattering angle θ_2 and ejection angle θ_1. Continuous curve, present calculation; dashed curve, first Born calculation.

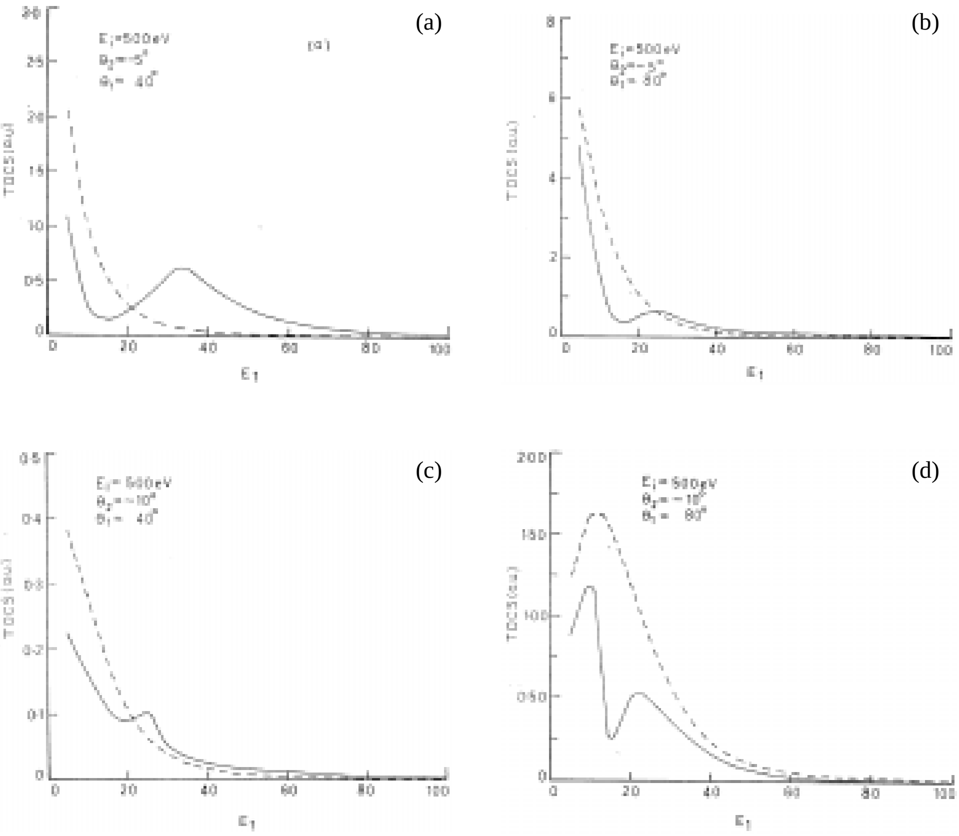

Figure 2a–d. Same as in figure 1, but for incident electron energy 500 eV.

Next we note that the experimental results of Schüle and Nakel [6] for Ag-atoms at a relativistic energy of 500 keV for the incident electron show somewhat similar pattern as those of the present calculation.

We further note that the energy spectra as obtained from the first Born calculation over the entire energy range, 5 eV–100 eV for the ejected electron, considered here, are very different.

To trace the physical origin of the peaks around two to three Rydbergs of energy, we consider different components of the scattering amplitude. Table 1 presents one such illustrative example. Here amplitude f_{PWB} corresponds to fourth term in the wave function eq. (2b), where both the outgoing electrons are described by plane waves. Similarly f_{eT} (which is also the first Born amplitude) corresponds to the first term on the right hand side of eq. (2b) in which the scattered electron (P) is described by a plane wave while the ejected electron (e) is described by a Coulomb wave. f_{PT} is similar to f_{eT}, except that the role of atomic electron and projectile electron is interchanged. For f_{Pe}, due to the third term on the right hand side of (2b), the projectile–electron interaction is treated exactly. A glance at table 1 shows that at around 20 eV, in this case, the amplitude f_{Pe} is substantially

Table 1. Different components of the scattering amplitude for ionization of hydrogen atoms by electrons of incident energy 250 eV for various ejected electron energies, for our present calculation (eq. (4a)) and for scattering angle $\theta_2 = -10^\circ$ and ejection angle $\theta_1 = 40^\circ$, scattering taking place in a plane.

E_1 (eV)	f_{PWB}	$f_{eT}(= f_B)$	f_{PT}	f_{Pe}
5	-0.548	$-0.839 + 1.212i$	$-0.147 + 0.006i$	$-0.710 - 0.054i$
10	-0.977	$-0.792 + 0.532i$	$-0.525 + 0.160i$	$-1.146 - 0.298i$
15	-0.942	$-0.574 + 0.278i$	$-0.544 + 0.166i$	$-1.181 - 0.444i$
20	-0.796	$-0.412 + 0.163i$	$-0.473 + 0.132i$	$-1.192 - 0.640i$
25	-0.647	$-0.302 + 0.104i$	$-0.391 + 0.094i$	$-0.592 - 1.126i$
30	-0.521	$-0.227 + 0.071i$	$-0.319 + 0.063i$	$-0.169 - 0.764i$
35	-0.420	$-0.175 + 0.050i$	$-0.261 + 0.040i$	$-0.056 - 0.543i$
40	-0.342	$-0.137 + 0.037i$	$-0.214 + 0.023i$	$-0.007 - 0.405i$
50	-0.233	$-0.090 + 0.022i$	$-0.149 + 0.003i$	$0.030 - 0.247i$
60	-0.165	$-0.062 + 0.014i$	$-0.108 - 0.007i$	$0.040 - 0.163i$

large, in magnitude, compared to other amplitudes, such as f_B. This shows that around the peak, the projectile–electron interaction is most important in the final channel. So the physical origin of the peaks may be traced to the double scattering first by the atomic nucleus (or by the atomic electron) and subsequently a second time by the atomic electron. Such peaks are also expected in second Born results or in BBK theory, but are absent in the first Born results.

4. Conclusions

The energy spectrum of the ejected electrons in electron hydrogen atom ionization collisions as calculated by the multiple scattering theory of Das and Seal shows interesting features which warrant experimental verification. Results of the present calculation differ drastically from the first Born results. Physical origin of the peaks are traced to double scattering effect, first scattering by atomic nucleus or atomic electron and then a second time by the atomic electron. Calculations for these cases by other familiar methods will also be interesting. Calculations with additional approximations have already been done [16] in case of ionization of Ag atom and the results are in good agreement with the experimental results of Schüle and Nakel [6]. Similar studies may be undertaken for many-electron lighter atoms as well.

References

[1] J N Das, *Il. Nuovo Cimento* **B12**, 197 (1972)
[2] D H Madison and E Merzbacher, *Atomic inner-shell processes* edited by B Crazemann (New York, Academic Press, 1975) p. 1
[3] J N Das and S Chakraborty, *Phys. Rev.* **A32**, 176 (1985)
[4] D H Jakubasa-Amundsen, *Z. Phys.* **D11**, 305 (1989); *J. Phys.* **B25**, 1297 (1992)
[5] S Keller, R M Dreizler, L U Ancarni, H R J Watters, H Ast and C T Whelan, *Z. Phys.* **D37**, 191 (1996)

[6] E Schüle and W Nakel, *J. Phys.* **B15**, L639 (1982)
[7] H Ruoff and W Nakel, *J. Phys.* **B20**, 2299 (1987)
[8] J Bonfert, H Graf and W Nakel, *J. Phys.* **B24**, 1423 (1991)
[9] H Ehrhardt, K Jung, G Knoth and P Schlemmer, *Z. Phys.* **D1**, 3 (1986)
[10] T D Mark, G H Dunn (eds), *Electron impact ionization* (Springer, New York, 1985)
[11] F W Byron and C J Joachain, *Phys. Rep.* **179**, 211 (1989)
[12] M Brauner, J S Briggs and H Klar, *J. Phys.* **B22**, 2265 (1989)
M Brauner, J S Briggs, H Klar, J T Board, T Rösel, K Jung and H Ehrhardt, *J. Phys.* **B24**, 657 (1991)
[13] A Lahmann-Bennani, *J. Phys.* **B24**, 2401 (1991)
[14] N F Mott and H S W Massey, *The theory of atomic collisions*, 4th ed. (Oxford, 1965) p. 492
[15] J N Das and S Seal, *Phys. Rev.* **A47**, 2978 (1993); see also *Pramana – J. Phys.* **40**, 253 (1993); *Z. Phys.* **D31**, 167 (1994); *Aust. J. Phys.* **47**, 49 (1994)
[16] J N Das and S Dhar, *J. Phys.* **B31**, 2355 (1998)