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STRUCTURE IN THE DIFFERENTIAL CROSS SECTIONS FOR THE EXCITATION OF 1 s^2 $S^e \rightarrow 2$ s^2 S^e TRANSITION IN H BY ELECTRON IMPACT AT 1 RYDBERG

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We have calculated the differential cross sections for the excitation 1 s^2 $S^e \rightarrow 2$ s^2 S^e transition in the hydrogen atomic system by electron impact using the basis functions (1s-2s-2p) within the R-matrix method at an incident energy 1 Rydberg. Our investigation demonstrates the structure in the differential cross section curve.

1. Introduction

The study of the scattering by the atomic hydrogen has been of growing interest in atomic collision physics, especially from the theoretical point of view, because the hydrogen atom provides an excellent testing ground for a theoretical model as the wave functions of both discrete and continuum states are exactly known. Consequently, the collision problem is not complicated by the atomic structure problem. The electron scattering by the atomic hydrogen is a three-body Coulomb problem treating a proton and two electrons. Although two-body Coulomb problem can be solved exactly, the exact solutions to the three-body Coulomb system are

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impossible to obtain. A number of approximate theoretical models to electron-atom scattering problems have been introduced in the literature which are applicable in different incident energy ranges (low, intermediate and high). The success or failure of these methods leads us to a better understanding of the problems that are encountered in other complex collision systems.

Great theoretical[1−27] and experimental[28−31] advancement has been made to solve the electron-hydrogen scattering problem in the very wide impact energy range. However, considerable discrepancy exists in the intermediate energy range where infinite number of bound and continuum channels are open. Effects due to other channels become important as the energy decreases towards the ionization threshold.

In the low bombarding energy region, the close-coupling (CC)[1] and the R-matrix[2−4] methods yield reliable results. In our present work, we have employed the standard R-matrix method with the basis functions (1s-2s-2p) exactly in the same way as in our earlier work[5−12] to calculate the electron impact angular differential cross sections for the excitation 1 s^2 S^e $\rightarrow$ 2 s^2 S^e optically forbidden transition in the hydrogen atom at alow incident energy of 1 Rydberg (1 Ry = 13.6 eV), 31 partial waves have been included. At an incident energy of 1 Ry, which is the ionization threshold of the hydrogen atom, one may not expect the standard R-matrix to be very reliable. However, in the absence of reliable theoretical predictions and experimental observations, our present results may give us some indication of the shape and qualitative features of the cross sections curve. In addition, this will provide a standard against by which later more accurate calculations can be judged.

2. *Calculation and results*

The wave functions describing the electron and the atomic system are represented by

$$\Psi_k = A \sum_{ij} a_{ijk} \Phi_i U_j + \sum_j b_{jk} \Phi_j \, , \qquad (1)$$

where Φ_i are channel functions, U_j are continuum basis orbitals and Φ_j are bound configurations formed from the atomic orbitals. The coefficients a_{ijk} and b_{jk} are obtained by diagonalising the total Hamiltonian in the basis defined in equation (1).

Figure 1 displays the electron impact angular differential cross sections ($a_0^2 Sr^{-1}$) for the excitation 1 s^2 S^e $\rightarrow$ 2 s^2 S^e optically forbidden transition, calculated using the R-matrix method with the basis functions (ls-2s-2p), in the atomic hydrogen at a low incident energy of 1 Ry together with available relevant theoretical results of van de Ree[11]. Several features of importance emerge from the Fig. 1. First, it is seen from the figure that there is a qualitative as well as quantitative difference between our curve 1 and the van de Ree curve 2. In the small scattering angular range of $\theta = 0°$ to $\theta \approx 28°$, our curve 1 lies above the van de Ree curve 2. From the scattering angle $\theta \approx 28°$ to $\theta = 180°$, our curve lies below the van de Ree curve 2. Second, our curve 1 clearly shows pronounced oscillations whereas the van de Ree curve 2 exhibits very weak oscillations. Our results show a deep minimum at around $\theta \approx 52°$ while the van de Ree curve is smoothly decaying up to $\theta \approx 69°$. The position of the broad maximum at around $\theta \approx 70°$ in our curve is very close to the shallow minimum of the van de Ree curve. The present R-matrix result produces a shallow minimum at around $\theta \approx 94°$ whereas the van de Ree curve does not exhibit such behaviour. Finally, in the backward scattering region, the inspection of the figure shows that there is a qualitative agreement between our curve 1 and the van de Ree curve 2.

3. Conclusion

It would be interesting to examine both experimentally and theoretically our predicted deep minimum, broad maximum, and shallow minimum in the differential cross sections curve.

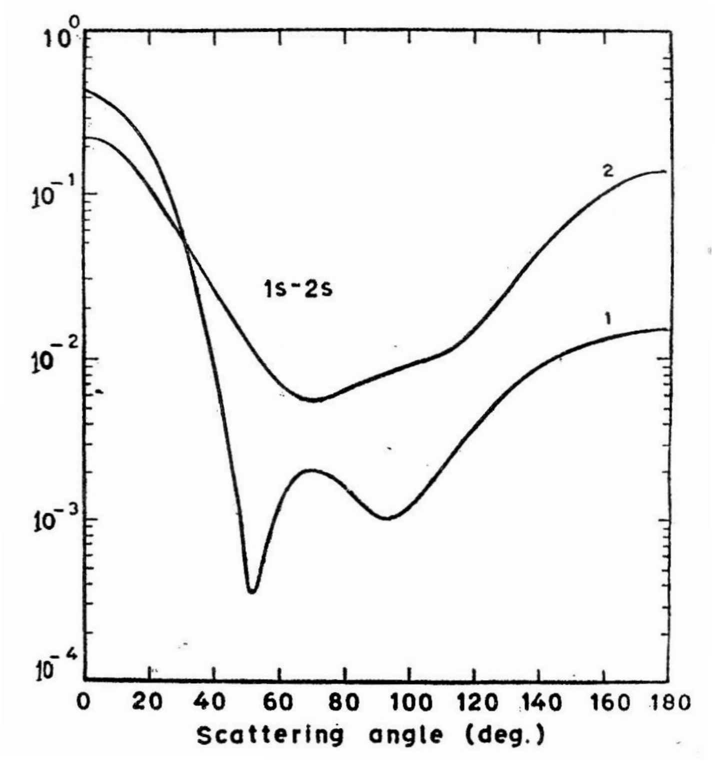

Fig. 1. Differential cross sections ($a_0^2 Sr^{-1}$) for the inelastic scattering process $e^- + H(1s) \rightarrow e^- + H(2s)$ *at an incident energy of 1 Ry. Curve 2 are van de Ree results.*

TABLE 1.

	ANGULAR DISTRIBUTION		
	THETA (DEGREES)	ANG. DISTR. (AU)	ANG. DISTR. (cm^2)
1	1.0000	0.44167138D+00	0.12367594D-16
2	2.0000	0.43872776D+00	0.12285167D-16
3	3.0000	0.43386695D+00	0.12149056D-16
4	4.0000	0.42715560D+00	0.11961126D-16
5	5.0000	0.41868468D+00	0.11723925D-16
6	6.0000	0.40856724D+00	0.11440618D-16
7	7.0000	0.39693572D+00	0.11114915D-16
8	8.0000	0.38393883D+00	0.10750978D-16
9	9.0000	0.36973818D+00	0.10353334D-16
10	10.0000	0.35450477D+00	0.99267715D-17
11	11.0000	0.33841541D+00	0.94762406D-17
12	12.0000	0.32164924D+00	0.90067576D-17
13	13.0000	0.30438437D+00	0.85233101D-17
14	14.0000	0.28679483D+00	0.80307713D-17
15	15.0000	0.26904780D+00	0.75338226D-17
16	16.0000	0.25130123D+00	0.70368868D-17
17	17.0000	0.23370186D+00	0.65440727D-17
18	18.0000	0.21638364D+00	0.60591315D-17
19	19.0000	0.19946662D+00	0.55854243D-17
20	20.0000	0.18305616D+00	0.51259019D-17
21	21.0000	0.16724261D+00	0.46830941D-17
22	22.0000	0.15210129D+00	0.42591099D-17
23	23.0000	0.13769276D+00	0.38556452D-17
24	24.0000	0.12406339D+00	0.34739983D-17
25	25.0000	0.11124612D+00	0.31150915D-17
26	26.0000	0.99261366D-01	0.27794969D-17
27	27.0000	0.88118138D-01	0.24674665D-17
28	28.0000	0.77815129D-01	0.21789637D-17
29	29.0000	0.68341934D-01	0.19136972D-17
30	30.0000	0.59680242D-01	0.16711542D-17
31	31.0000	0.51805034D-01	0.14506342D-17
32	32.0000	0.44685732D-01	0.12512809D-17
33	33.0000	0.38287295D-01	0.10721132D-17
34	34.0000	0.32571251D-01	0.91205367D-18
35	35.0000	0.27496638D-01	0.76995536D-18
36	36.0000	0.23020862D-01	0.64462558D-18
37	37.0000	0.19100469D-01	0.53484751D-18
38	38.0000	0.15691813D-01	0.43939900D-18
39	39.0000	0.12751645D-01	0.35706902D-18
40	40.0000	0.10237608D-01	0.28667146D-18
41	41.0000	0.81086483D-02	0.22705675D-18
42	42.0000	0.63253492D-02	0.17712116D-18
43	43.0000	0.48501957D-02	0.13581421D-18
44	44.0000	0.36477701D-02	0.10214413D-18
45	45.0000	0.26848908D-02	0.75181776D-19
46	46.0000	0.19306985D-02	0.54063034D-19
47	47.0000	0.13566978D-02	0.37989980D-19
48	48.0000	0.93675926D-03	0.26230946D-19
49	49.0000	0.64708933D-03	0.18119666D-19

Table 1. (cont.)

50	50.0000	0.46617232D-03	0.13053664D-19
51	51.0000	0.37469076D-03	0.10492016D-19
52	52.0000	0.35542806D-03	0.99526255D-20
53	53.0000	0.39315816D-03	0.11009136D-19
54	54.0000	0.47452549D-03	0.13287568D-19
55	55.0000	0.58791889D-03	0.16462787D-19
56	56.0000	0.72334195D-03	0.20254876D-19
57	57.0000	0.87228247D-03	0.24425479D-19
58	58.0000	0.10275829D-02	0.28774170D-19
59	59.0000	0.11833134D-02	0.33134905D-19
60	60.0000	0.13346492D-02	0.37372579D-19
61	61.0000	0.14777525D-02	0.41379730D-19
62	62.0000	0.16096613D-02	0.45073415D-19
63	63.0000	0.17281836D-02	0.48392252D-19
64	64.0000	0.18317992D-02	0.51293674D-19
65	65.0000	0.19195684D-02	0.53751370D-19
66	66.0000	0.19910483D-02	0.55752936D-19
67	67.0000	0.20462156D-02	0.57297719D-19
68	68.0000	0.20853968D-02	0.58394865D-19
69	69.0000	0.21092058D-02	0.59061560D-19
70	70.0000	0.21184869D-02	0.59321445D-19
71	71.0000	0.21142648D-02	0.59203219D-19
72	72.0000	0.20977006D-02	0.58739393D-19
73	73.0000	0.20700532D-02	0.57965214D-19
74	74.0000	0.20326450D-02	0.56917718D-19
75	75.0000	0.19868338D-02	0.55634923D-19
76	76.0000	0.19339879D-02	0.54155142D-19
77	77.0000	0.18754653D-02	0.52516405D-19
78	78.0000	0.18125971D-02	0.50755982D-19
79	79.0000	0.17466732D-02	0.48909992D-19
80	80.0000	0.16789313D-02	0.47013099D-19
81	81.0000	0.16105488D-02	0.45098266D-19
82	82.0000	0.15426360D-02	0.43196584D-19
83	83.0000	0.14762317D-02	0.41337145D-19
84	84.0000	0.14123010D-02	0.39546969D-19
85	85.0000	0.13517331D-02	0.37850961D-19
86	86.0000	0.12953421D-02	0.36271910D-19
87	87.0000	0.12438669D-02	0.34830512D-19
88	88.0000	0.11979736D-02	0.33545416D-19
89	89.0000	0.11582572D-02	0.32433285D-19
90	90.0000	0.11252448D-02	0.31508879D-19
91	91.0000	0.10993986D-02	0.30785139D-19
92	92.0000	0.10811192D-02	0.30273283D-19
93	93.0000	0.10707494D-02	0.29982911D-19
94	94.0000	0.10685779D-02	0.29922106D-19
95	95.0000	0.10748428D-02	0.30097533D-19
96	96.0000	0.10897354D-02	0.30514552D-19
97	97.0000	0.11134038D-02	0.31177310D-19
98	98.0000	0.11459563D-02	0.32088840D-19
99	99.0000	0.11874650D-02	0.33251159D-19
100	100.0000	0.12379686D-02	0.34665349D-19
101	101.0000	0.12974753D-02	0.36331645D-19
102	102.0000	0.13659661D-02	0.38249510D-19

Table 1. (cont.)

103	103.0000	0.14433968D-02	0.40417708D-19
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106	106.0000	0.17285596D-02	0.48402780D-19
107	107.0000	0.18408863D-02	0.51548130D-19
108	108.0000	0.19616323D-02	0.54929237D-19
109	109.0000	0.20906459D-02	0.58541849D-19
110	110.0000	0.22277626D-02	0.62381362D-19
111	111.0000	0.23728063D-02	0.66442847D-19
112	112.0000	0.25255904D-02	0.70721076D-19
113	113.0000	0.26859183D-02	0.75210547D-19
114	114.0000	0.28535843D-02	0.79905498D-19
115	115.0000	0.30283742D-02	0.84799930D-19
116	116.0000	0.32100656D-02	0.89887614D-19
117	117.0000	0.33984282D-02	0.95162107D-19
118	118.0000	0.35932247D-02	0.10061676D-18
119	119.0000	0.37942107D-02	0.10624473D-18
120	120.0000	0.40011347D-02	0.11203897D-18
121	121.0000	0.42137388D-02	0.11799227D-18
122	122.0000	0.44317586D-02	0.12409722D-18
123	123.0000	0.46549234D-02	0.13034624D-18
124	124.0000	0.48829565D-02	0.13673157D-18
125	125.0000	0.51155748D-02	0.14324530D-18
126	126.0000	0.53524898D-02	0.14987935D-18
127	127.0000	0.55934068D-02	0.15662546D-18
128	128.0000	0.58380257D-02	0.16347523D-18
129	129.0000	0.60860410D-02	0.17042010D-18
130	130.0000	0.63371418D-02	0.17745138D-18
131	131.0000	0.65910121D-02	0.18456020D-18
132	132.0000	0.68473310D-02	0.19173759D-18
133	133.0000	0.71057732D-02	0.19897444D-18
134	134.0000	0.73660087D-02	0.20626150D-18
135	135.0000	0.76277035D-02	0.21358943D-18
136	136.0000	0.78905199D-02	0.22094876D-18
137	137.0000	0.81541167D-02	0.22832994D-18
138	138.0000	0.84181494D-02	0.23572334D-18
139	139.0000	0.86822711D-02	0.24311922D-18
140	140.0000	0.89461323D-02	0.25050781D-18
141	141.0000	0.92093819D-02	0.25787927D-18
142	142.0000	0.94716673D-02	0.26522373D-18
143	143.0000	0.97326347D-02	0.27253129D-18
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146	146.0000	0.10504090D-01	0.29413344D-18
147	147.0000	0.10756249D-01	0.30119434D-18
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149	149.0000	0.11250973D-01	0.31504749D-18
150	150.0000	0.11492844D-01	0.32182031D-18
151	151.0000	0.11730597D-01	0.32847783D-18
152	152.0000	0.11963895D-01	0.33501059D-18
153	153.0000	0.12192403D-01	0.34140924D-18
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Table 1. (cont.)

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159	159.0000	0.13444948D-01	0.37648275D-18
160	160.0000	0.13631111D-01	0.38169564D-18
161	161.0000	0.13810054D-01	0.38670636D-18
162	162.0000	0.13981511D-01	0.39150748D-18
163	163.0000	0.14145228D-01	0.39609184D-18
164	164.0000	0.14300959D-01	0.40045260D-18
165	165.0000	0.14448471D-01	0.40458320D-18
166	166.0000	0.14587543D-01	0.40847745D-18
167	167.0000	0.14717963D-01	0.41212947D-18
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169	169.0000	0.14952078D-01	0.41868511D-18
170	170.0000	0.15055417D-01	0.42157879D-18
171	171.0000	0.15149397D-01	0.42421038D-18
172	172.0000	0.15233874D-01	0.42657588D-18
173	173.0000	0.15308719D-01	0.42867168D-18
174	174.0000	0.15373818D-01	0.43049457D-18
175	175.0000	0.15429071D-01	0.43204177D-18
176	176.0000	0.15474395D-01	0.43331090D-18
177	177.0000	0.15509719D-01	0.43430004D-18
178	178.0000	0.15534989D-01	0.43500765D-18
179	179.0000	0.15550166D-01	0.43543265D-18
180	180.0000	0.15555228D-01	0.43557438D-18

Complete presentation of the results of our present calculation for the cross sections as a function of scattering angle at an incident energy 13.6eV.

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STRUKTURA U DIFERENCIJALNOM UDARNOM PRESJEKU ZA POBUĐ ENJE PRIJELAZA 1 s^2 $S^e \to 2$ s^2 S^e U H SUDAROM ELEKTRONA ENERGIJE 1 Ry

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Originalni znanstveni rad

Izračunali smo diferencijalni udarni presjek za pobuđenje prijelaza 1 s^2 $S^e \to 2$ s^2 S^e u vodikovom atomu sudarom elektrona energije 1 Rydberg. Koristili smo bazu funkcija (ls-2s-2p) u R-matričnoj metodi. Naše istraživanje otkriva da krivulja diferencijalnog udarnog presjeka posjeduje strukturu.