

ELECTRON COLLISION WITH CAESIUM ATOM

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ABSTRACT. The elastic scattering cross section for slow electron scattering by caesium atom has been calculated by taking the form of Stone and Reitz for the atomic potential and that of Biermann and Harting for the polarization potential. As the exchange effect is negligible in the energy corresponding $K^2 = 1$ a.u., its consideration has been excluded.

I N T R O D U C T I O N

In the study of the elastic scattering of slow electron by neutral atom we are up against the difficulty of the choice of a suitable potential to represent the field generated by the nucleus and the surrounding electrons of the atom; further we have to consider the distortion of this field induced by the incoming electron. In such a calculation we have to bear in mind the possibility of exchange of roles between the incoming electron and the bound electron when they are close to each other during the impact. Salmona and Seaton (1960) have calculated such a process in Bethe approximation for sodium and caesium atoms and have found that the value of the cross section for Cs. atom reaches a maximum at an energy value $K^2 = .09$ atomic units, which is nearly the same as has been found experimentally by Brode (1929), but the magnitude of the cross section at that energy is much less than that of Brode. Garrett and Mann (1963) have taken the potential for the atomic field of Cs. atom due to Hartree and for the polarization field due to Biermann and Harting (1942); except for a little increase in the region $.04 < K^2$

$.06$ a.u. their cross section decreases monotonously with the increase of energy in the range $.01 < K^2 < 1.96$ a.u. Their calculation fails to show the sharp peak at $K^2 = .09$ a.u. as observed experimentally by Brode. Stone and Reitz (1963) using an adiabatic model and including exchange effect have calculated the cross section of scattering in the region $.00025 < K^2 < .065$ a.u. They have found that the influence of exchange is quite considerable below $K^2 = .02$ a.u. and is small thereafter. The variation of cross section with energy in that range shows a maximum at the value $K^2 = .02$ a.u. However, the experimental results of Chen and Raether (1962) do not agree with their calculated values. Using a first order perturbation theory in the adiabatic approximation Crown and Russek (1965) have calculated the same problem in the energy range $.00005 < K^2 < <2$ a.u. They have obtained a minimum value for the scattering cross section

at $K^2 = .0085$ a.u., whereas Stone and Reitz (1963) have obtained a maximum value near about the same point

In view of the fact that the theoretical results are at variance with each other we have made an attempt to calculate the same problem taking different combination of potentials with a view to obtaining better fit with experimental results, which are also not quite consistent. For our calculation we have chosen the potential field of the Cs. atom as that of Stone and Reitz (1963) and the polarization potential of Biermann and Harting (1942). The value of the scattering cross section in units of πa_0^2 at the energy $K^2 = 1$ a.u. comes to 407 as compared to 160 of Garrett and Mann (1963) and 70 of Crown and Russek (1965), whereas the experimental value due to Brode (1929) is 263

The potential for the screened atomic field of Cs. is split up into two parts. For the region $0 < r < 2$ a.u. we take the form of Prokofjew which is a modification of the Hartree potential for Cs^+ ion, and which has been tabulated by Stone (1962) for the values of the effective charge $Z(r)$ of the Cs^+ ion core against r . We are justified in taking this potential because inner core electrons are insensitive to the state of the valence electron. In the region $2 < r < \infty$ we choose the values given by Stone and Reitz (1963) who had plotted the logarithm of the potential $V(r)$ against r . As this curve is a straight line we choose $V = Ae^{-br}$. Our potential is continuous at $r = 2$. For the polarization potential we use the form of Biermann and Harting which has also been used by Garrett and Mann in their calculation.

$$Vp = \frac{\alpha}{2r^4} \left[1 - \exp \left\{ - \left(\frac{r}{\sqrt{r_0}} \right)^6 \right\} \right]$$

where α is the polarizability of the atom

As the influence of exchange is not of considerable value at $K^2 = 1$ a.u. (27.2 e.v.), we have not included it in our present calculation.

T H E O R Y

The differential cross section is given by

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{K^2} \left| \sum_{l=0}^{\infty} (2l+1)e^{i\eta_l} \sin \eta_l p_l(\cos \theta) \right|^2$$

The total cross section becomes

$$\sigma = \sum_l \sigma_l$$

where

$$\sigma_l = \frac{4\pi}{K^2} (2l+1) \sin^2 \eta_l$$

To calculate the phase shift η_l we have used WKB method with Langer modification, according to which the phase shift is given by (c.f. Landau and Lifshits, 1959)

$$\eta_l = \int_{r_l}^{\infty} \left[\frac{1}{\hbar} \left\{ 2m(E-U) - \frac{\hbar^2(l+\frac{1}{2})^2}{r^2} \right\}^{\frac{1}{2}} - K \right] dr + \frac{\pi(l+\frac{1}{2})}{2} - Kr_l$$

where r_l is the value of r for which the expression under the radical sign is zero.

RESULTS AND DISCUSSIONS

The potential term U consists of two parts; one due to the field of the Cs. atom and the other due to the polarization induced by the incident electron.

$$-U = V(r) + V_p(r).$$

$$V(r) = \frac{Z(r)}{r} \quad \text{for } 0 < r \leq 2$$

$$= 2.2594e^{-3r} \quad \text{for } 2 \leq r < \infty$$

$$V_p(r) = \frac{\alpha}{2r^4} \left[1 - \exp \left\{ - \left(\frac{r}{f_0} \right)^6 \right\} \right]$$

We have taken

$$\alpha = 243 \text{ atomic units}$$

$$r_0 = 6.13 \text{ atomic units}$$

$$f = .8$$

Using the above values of the parameters we have numerically integrated the expression

$$\int_{r_l}^{\infty} \frac{1}{\hbar} \left\{ 2m(E-U) - \frac{\hbar^2(l+\frac{1}{2})^2}{r^2} \right\}^{\frac{1}{2}} - K \right\} dr$$

From Table I it can be seen that at the incident energy $K^2 = 1$ a.u. quite a large number of phase shifts contributes appreciably to the total cross section. The contribution from such a large number of phase shifts has considerably increased the value of the total cross section σ . The value of the total cross section obtained by us at $K^2 = 1$ a.u. in units of πa_0^2 is 407, the same obtained by Garrett and Mann is 160 and by Crown and Russek is 76; whereas the experimental value due to Brode is 263 at that energy. It may be mentioned here that at our energy the influence of polarization potential is not of much consequence. The value

TABLE I

Calculated phase shifts and partial cross sections at $K^2 = 1$ a.u.
(27.2 e.v.)

l	η_l	σ_l in the units of πa_0^2
0	18 220	1.36
1	17 955	7 30
2	12 648	0.13
3	6 635	3.32
4	4 505	34 47
5	3 901	20 48
6	3 653	12.46
7	2 824	5.84
8	2 247	41.35
9	1 207	66 38
10	1.009	60.19
11	0 867	53 46
12	0.638	35.52
13	0.491	24.03
14	0.374	15.47
15	0 273	9.04
16	0.269	9.37
17	0.173	4.17
18	0 117	2 03

obtained by Garrett and Mann with Hartree potential is less than the experimental value of Brode, the potential of Stone and Reitz extends further than the Hartree field, as such we felt that the potential of Stone and Reitz would increase the value of the cross section to bring it in better agreement with the experimental value, but the increase is much more than our expectations. It is difficult to judge the suitability of this potential by calculating the cross section at one energy, for proper appraisal it is necessary to see its variation with energy. It is not easy to reconcile our too large value with the too low value of Crown and Russek, who have, in support of their result, compared with the experimental value of Margulis and Korchevoi (1962), which differs considerably from that of Brode (Margulis and Korchevoi have obtained 57 for $K^2 = .048$ whereas the value of Brode is 300 for nearly the same point).

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