CROSS SECTION FORMULAE FOR IONIZATION AND EXCITATION OF ATOMS BY HIGH ENERGY ELECTRONS

by B. L. SCHRAM

FOM-Laboratorium voor Massascheiding, Amsterdam, Nederland

and L. VRIENS

Fysisch Laboratorium der Universiteit, Utrecht, Nederland

Synopsis

In the Bethe-Born approximation the cross sections for ionization or excitation of atoms by electrons of high energy E_1, are given by $\sigma = A/E_1 \ln cE_1$ for optically allowed transitions and by $\sigma = B/E_1$ for disallowed transitions. Here A, B and c are constants for a given transition. For ionization or excitation processes to which both types of transitions contribute, the total cross sections are given by

$$\sigma = \frac{A}{E_1} \ln cE_1 + \frac{B}{E_1} = \frac{A}{E_1} \ln c'E_1.$$

These formulae are frequently simplified using the approximation $cU \approx c'U \approx 4$, where U is the ionization or excitation energy. It is shown that great deviations from these latter approximations occur.

Introduction. In the present article, we discuss two approximations usually made in cross section formulae for ionization and excitation of atoms by high energy electrons. For simplicity, we firstly restrict ourselves to excitation, and next generalize the problem to ionization.

In the first Born approximation, the differential cross section for momentum change $\hbar K$ in excitation of an atom from state n to state n' is[1])

$$\sigma(K) \, dK = \frac{8\pi a_0^2 R^2}{E_1 U} f(K) \, \frac{dK}{K}, \tag{1}$$

where a_0 is the radius of the first Bohr orbit of atomic hydrogen, R is the Rydberg energy (13.595 eV), U is the excitation energy, E_1 is the electron energy and $f(K)$ is the generalized oscillator strength of Bethe[2]),

$$f(K) = \frac{U}{R} \left| \frac{1}{Ka_0} \langle n' | e^{iKx} | n \rangle \right|^2, \tag{2}$$

where

$$\langle n' | e^{iKx} | n \rangle = \int \psi_{n'}^* \, e^{iKx} \, \psi_n \, d\tau$$

in which $\psi_{n'}$ is the final state wave function and ψ_n is the initial state wave function of the atom. As for many transitions, the small momentum transfers are the most important ones, it is convenient to expand e^{iKx} in a power series in which the first term vanishes because of the orthogonality of the wave functions, so that

$$f(K) = \frac{U}{R} \left| \frac{1}{Ka_0} \sum_{s=1}^{\infty} \frac{(iK)^s}{s!} \langle n' |x^s| n \rangle \right|^2, \tag{3}$$

where $\langle n' |x| n \rangle$ is the dipole (length) matrix element and

$$\lim_{K \to 0} f(K) = \frac{U}{R} \left| \frac{\langle n' |x| n \rangle}{a_0} \right|^2 = f$$

where f is the optical oscillator strength.

Excitation cross sections are obtained by integrating (1) over the possible values of K, determined by the law of conservation of momentum.

For an optically allowed transition this gives[1][3])

$$\sigma = \frac{A}{E_1} \ln cE_1 \tag{4}$$

where

$$A = \frac{4\pi a_0^2 R^2}{U} f \text{ and } \frac{cU^2}{4R} = \frac{K_{cd}^2 a_0^2}{(2E_1/U)^2 [1 - (1 - U/E_1)^{\frac{1}{2}}]^2}$$

in which K_{cd} is the momentum cutoff factor for dipole transitions[3])[4]). For large E_1 this last relation can be simplified to

$$\frac{cU^2}{4R} = K_{cd}^2 a_0^2.$$

The physical meaning of c or K_{cd} will be clear if $f(K)$ is plotted against $\ln(K^2 a_0^2)$ such as is done in ref. 5.

For an optically disallowed quadrupole transition, the first term ($s = 1$) in (3) vanishes and

$$\lim_{K \to 0} \frac{f(K)}{K^2 a_0^2} = \frac{U}{4R} \left| \frac{\langle n' |x^2| n \rangle}{a_0^2} \right|^2$$

where $\langle n' |x^2| n \rangle$ is the quadrupole matrix element.

Integration of (1) then leads to

$$\sigma = \frac{B}{E_1} \tag{5}$$

where

$$B = \pi a_0^2 R \left| \frac{\langle n' |x^2| n \rangle}{a_0^2} \right|^2 \left(K_{cq}^2 a_0^2 - \frac{E_1}{R} \left[1 - \left(1 - \frac{U}{E_1} \right)^{\frac{1}{2}} \right]^2 \right) \tag{6}$$

which for large E_1 reduces to:

$$B = \pi a_0^2 R \left| \frac{\langle n' \, |x^2| \, n \rangle}{a_0^2} \right|^2 (K_{cq}^2 a_0^2).$$

The physical meaning of momentum cutoff factor K_{cq} for a quadrupole transition will be clear if $f(K)/K^2 a_0^2$ is plotted against $K^2 a_0^2$. This gives similar curves as given in refs. 1 and 5 for a dipole transition.

For ionization of atoms, Rf/U in A and $\langle n' \, |x^2| \, n \rangle$ in B are replaced by analogous quantities, e.g. Rf/U by M_i^2, where M_i^2 is defined in ref. 1.

We note that A and B as used in this paper, are not equal to the Einstein coefficients for spontaneous emission and absorption.

Application to cross section calculations. To show how (4) and (5) can be used, we give two examples. First we consider excitation of atomic hydrogen from the ground state to the $n' = 2$ states $(2s, 2p)$. Then (4) gives the cross section for 1s $\rightarrow$ 2p and (5) gives the cross section for 1s $\rightarrow$ 2s. Hence the total cross section for $1s \rightarrow 2(s + p)$ is given by

$$\sigma = \frac{A}{E_1} \ln cE_1 + \frac{B}{E_1}. \tag{7}$$

An alternative expression for (7) is:

$$\sigma = \frac{A}{E_1} \ln c'E_1 \tag{8}$$

with $c' = c \exp (B/A)$.

Secondly we consider ionization of atomic hydrogen from the ground state. Then (4) gives the partial cross section for ejection of the atomic electron to a continuum p state, (5) gives the partial cross section for ejection of the atomic electron to continuum s, d, f, g, ... states, and (7) gives the total cross section. We note that (6) is only valid for quadrupole transitions, but, as all higher order multipole transitions also give cross sections which are proportional to E_1^{-1}, we can include their contributions to the cross sections in the constant B.

The usual way to determine c or K_{cd} for any transition is to equate the Bethe expression (4) to calculated Born cross sections or known experimental cross sections (for large E_1).

This method is correct when one has to do exclusively with dipole transitions. If, however, optically disallowed transitions are contributing to the total cross sections, it can be seen from (8) that one determines c' instead of c.

Measurements of excitation cross sections commonly give the partial (allowed or disallowed) cross sections; calculations of excitation cross sections are performed both for partial and total (allowed + disallowed)

cross sections. Measurements of ionization cross sections always give the total cross sections; many calculations for ionization are also performed only for the total cross sections.

In some books on atomic collision theories [6] (4), (7) and (8) are simplified to

$$\sigma = \frac{A}{E_1} \ln 4 \frac{E_1}{U}. \tag{9}$$

This simplification is commonly justified by the following:
1. In general, the dipole transitions give larger contributions to the total cross sections than the disallowed transitions. Moreover, (4) falls of more slowly with large E_1 than (5). Hence, for sufficiently large E_1 the disallowed transitions can be neglected and (4) gives the correct high energy limit both for partial dipole and total cross sections.
2. For sufficiently large E_1 the exact value of c is not very important. Further, cU is not very different for various transitions (or $K_{cd}a_0 \sim \sqrt{U}$) and assumed to be approximately equal to 4.

Some objections can be made against these two simplifications. First we note that cU can be considerably smaller than 4 for optically allowed excitation. For instance, $cU = 0.0979$ for the transition $10s \rightarrow 11p$ in atomic hydrogen [7]. Second, we remark that cU can be substantially smaller than $c'U$. As far as we know, many cU values for ionization of atoms lie between 1 and 4, so the approximation $cU \approx 4$ is reasonable for ionization. Hence the approximation $c'U \approx 4$ is only justified if for instance $B < A$. Recent calculations of Peach [8] show that the contributions of the disallowed transitions to the total ionization cross sections can be very important (e.g. for Li and Be), and recent calculations of one of us (L.V.) show that cU and $c'U$ values can be very different.

To demonstrate the influence of the disallowed transitions, we listed in table I values of cU and $c'U$. To the values previously reported [7], we added

TABLE I

Comparison of cU and c'U values			
Transition	cU	Transition	c'U
H 1s → 2p	1.23 (1.26)	H 1s → 2	1.49
H 1s → 3p	1.73	H 1s → 3	2.67
H 2s → 3p	0.510	H 2s → 3	2.99
		H 2p → 7	24.8
H 3s → 4p	0.328	H 3s → 4	3.42
H 10s → 11p	0.0979		
		H 1s → H⁺	77 (83)
H 2s → H⁺p	2.7	H 2s → H⁺	77
H 2p → H⁺(s + d)	3.5	H 2p → H⁺	26300
		He → He⁺	2.60
		H₂ → H₂⁺	4.33

a few calculated values of $c'U$ for excitation of atomic hydrogen from various levels and two experimentally determined values for the ionization of helium[9]) and molecular hydrogen[10]), where the value for helium has been corrected for the contribution of double ionization, which was not yet done in previous work[10]). The calculations were performed according to the procedure outlined before. The total Born cross sections used here are given by McCarroll[11]) (1s → 3, $E_1 = 982.24$ eV) Scanlon and Milford[12]) (2s → 3; $E_1 = 945.74$ eV), McCrea and McKirgan[13]) (2p → 7; $E_1 = 122,36$ eV) and McCoyd e.a.[14]) (3s → 4; $E_1 = 1361$ eV). For the transition 2p → 7 the factor A was taken equal to the sum for 2p → 7s and 2p → 7d.

Conclusions. From table I it clearly follows that the approximation $c'U \approx cU \approx 4$ can be a poor one. From measured total ionization cross sections[9][10]) and from calculated total ionization and excitation cross sections, only $A(M_i^2$ or $f)$ and $c'(c'U)$ values can be derived. If for instance only the dipole and quadrupole transitions are important, then

$$c'U = \frac{4RK_{cq}^2 a_0^2}{U[1 + (U/2E_1)]} \exp\left(\frac{K_{cq}^2 a_0^2 - (U^2/4E_1R)}{4M^2} \left|\frac{\langle n' |x^2| n\rangle}{a_0^2}\right|^2\right)$$

where M^2 is M_i^2 for ionization and is Rf/U for excitation. Hence the $c'U$ values cannot be correlated directly with the momentum cutoff factors. These factors and the cU values can only be derived from partial cross sections. As $c'U$ values can be very different and because (8) suggests a wrong momentum cutoff, we prefer the use of (7) above the use of (8). For this reason one of us (L.V.) previously called the cU values, derived from the partial cross sections, the correct ones[7]). For ionization the approximation $cU \approx 4$ inserted in (7) probably will be reasonable.

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