

APPROXIMATE CROSS SECTIONS FOR OPTICALLY DISALLOWED EXCITATION OF ATOMS BY ELECTRONS

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Synopsis

Formulae for approximate calculation of excitation cross sections for optically disallowed transitions are discussed. It is shown that the formula previously given by Drawin can be used in a different manner than pointed out by this author. This different manner seems to give reasonably accurate cross sections for small energies of the incident electrons, and gives the correct high energy limit. A comparison is made between approximate cross sections calculated here and already known Born cross sections.

Introduction. Knowledge of excitation and ionization cross sections of atoms is important in astrophysics and plasmaphysics. Experimentally determined cross sections are only available for a restricted number of transitions, in most cases only from the ground state. Theoretical calculations of cross sections are very complicated and have also been carried out only for a limited number of transitions. The results of such calculations are generally not very well in agreement with experiment for small energies of the impinging electrons. Approximate calculation of cross sections with simple empirical formulae often gives better results than complicated theoretical calculations. In previous papers we considered ionization and optically allowed excitation of atoms¹). In this paper we consider optically disallowed excitation of atoms without exchange. Hence we restrict ourselves here to transitions such as $H\ 1s \rightarrow 2s, 3s, 4s, 3d, 5f$; $H\ 2p \rightarrow 3p, 6f$; $He\ 1^1S \rightarrow 3^1S, 3^1D, 4^1D$; we neglect exchange in these transitions and do not consider transitions such as $He\ 1^1S \rightarrow 2^3S, 3^3P, 3^3D$.

Empirical formulae. Scanlon and Milford²) have given empirical formulae for quadrupole excitation. These formulae can be used for approximate calculation of cross sections for small electron energies E_1 , if the values of the cross section for two sufficiently large electron energies E_1 are known. Their formulae can also be used if the cross section for one sufficiently large electron energy E_1 and simultaneously the quadrupole matrix element are known. However, these authors pointed out themselves that

for several transitions in atomic hydrogen their formulae give cross sections as large as two to six times the Born cross sections for small E_1 . As it is much more probable that the Born approximation overestimates the cross sections for small E_1 than that it underestimates these cross sections (see for instance ref. 3), their empirical formulae do not seem to be very reliable.

Drawin⁴⁾ has given the following empirical formula for optically disallowed excitation without exchange

$$Q = Q_m \frac{4U}{E_1} \left(1 - \frac{U}{E_1} \right) \quad (1)$$

where U is the excitation energy and where he takes Q_m equal to the maximum experimental cross section. In this manner, (1) can only be used if Q_m is known experimentally. Absolute measurements of excitation cross sections in general are more difficult than relative measurements, which implies that if Q_m is known absolutely, the excitation function is also known absolutely. Then application of (1) in the manner as pointed out by Drawin, is only useful a, to obtain an estimate of the Q 's for large E_1 , b. for applications (e.g. if one wants to integrate over a Maxwellian electron energy distribution), c. to check the accuracy of (1). We note that theoretically calculated Q_m values are not very reliable, so that use of them in (1) is not advisable.

The function (1) can also be used in a different manner, for which purpose we replace $4Q_m U$ by B , so that

$$Q = \frac{B}{E_1} \left(1 - \frac{U}{E_1} \right) \quad (2)$$

where B is now chosen such that (2) gives the correct high energy limit (B is a constant for one transition; we note that our B is not related to the Einstein absorption probability). Hence, for application of (2) only one cross section for a sufficiently large value of $E_1 (\gg U)$ should be known; then the value of B for that transition can be found immediately.

Approximate cross sections. For a number of transitions in atomic hydrogen, Born cross sections for large and for small E_1 are calculated by Scanlon and Milford²⁾, and by McCoyd, Milford and Wahl⁵⁾. With their Q values for the largest E_1 values for which data are given (≈ 1 keV), we calculated B values, which for small E_1 were used for approximate calculation (eq. 2) of cross sections. In table I, the calculated B values are listed. In table II, the approximately (eq. 2) calculated cross sections for small E_1 are compared with Born cross sections given by Scanlon *e.a.* and McCoyd *e.a.*.

From table II it follows that for small E_1 , (2) gives smaller cross sections than the Born approximation gives. As already pointed out, this is more

TABLE I

Calculated B values for atomic hydrogen					
trans.	B (πa_0^2 eV)	trans.	B (πa_0^2 eV)	trans.	B (πa_0^2 eV)
1s \rightarrow 2s	6.02	2s \rightarrow 3d	228	3p \rightarrow 4p	368
1s \rightarrow 3s	1.20	2p \rightarrow 3p	79	3p \rightarrow 4f	717
2s \rightarrow 4s	14.1	3s \rightarrow 4s	311	3d \rightarrow 4s	7.40
2p \rightarrow 4f	21.1	3s \rightarrow 4d	636	3d \rightarrow 4d	295
2s \rightarrow 3s	72.2	3s \rightarrow 4f	324		

TABLE II

Comparison of Born cross sections ²⁾ ⁵⁾ and cross sections calculated with (2); for disallowed excitation of atomic hydrogen by electrons with energy E_1									
trans.	U (eV)	E_1 (eV)	Q Born (πa_0^2)	Q eq. (2) (πa_0^2)	trans	U (eV)	E_1 (eV)	Q Born (πa_0^2)	Q eq. (2) (πa_0^2)
1s \rightarrow 2s	10.196	13.34	0.246	0.106	3s \rightarrow 4s	0.661	0.7391	64	45
		17.32	0.242	0.143			0.9675	116	102
		26.67	0.186	0.140			3.256	78	76
1s \rightarrow 3s	12.084	13.60	0.037	0.0098	3s \rightarrow 4d	0.661	0.7391	120	91
		16.46	0.045	0.0193			0.9675	235	208
		19.82	0.044	0.0236			3.256	159	155
2s \rightarrow 4s	2.549	3.336	1.95	1.00	3s \rightarrow 4f	0.661	0.7391	270	46
		4.331	2.04	1.34			0.9675	290	106
		10.77	1.14	1.00			3.256	99	80
2p \rightarrow 4f	2.549	2.604	0.58	0.17	3p \rightarrow 4p	0.661	0.7391	83	53
		3.336	1.93	1.49			0.9675	145	120
		4.331	2.25	2.00			3.256	93	90
2s \rightarrow 3s	1.888	1.913	3.3	0.49	3p \rightarrow 4f	0.661	0.7391	290	103
		2.604	12.4	7.6			0.9675	394	235
		3.401	12.7	9.4			3.256	193	175
2s \rightarrow 3d	1.888	10.42	6.1	5.7	3d \rightarrow 4s	0.661	0.7391	3.3	1.06
		2.604	47	24			0.9675	4.22	2.43
		3.401	45	30			3.256	1.91	1.81
2p \rightarrow 3p	1.888	10.42	19.8	18	3d \rightarrow 4d	0.661	0.7391	100	42
		1.913	4.2	0.54			0.9675	146	97
		2.604	14.9	8.3			3.256	78	73
		3.401	14.8	10.3					
		10.42	6.8	6.2					

likely to be correct as the Born approximation in general overestimates the cross sections for small E_1 . For some transitions the discrepancies between Born approximation and (2) are large for very small E_1 (near threshold). As the electron exchange process can give considerable contributions to the cross sections for very small E_1 , (2) can underestimate the cross sections near threshold for some transitions. We should note that the Born approximation does not take account of exchange either. Further, Born approximation and (2) do not predict fine structure in the excitation functions near threshold as sometimes found in experiment⁶⁾. For completeness, we also have listed in table II Q values for very small E_1 . For $E_1 > 2U$, we believe that (2) will be reasonably accurate. Equations (1) and (2) predict that the

excitation functions reach a maximum for $E_1 = 2U$. For several transitions in He this is very well in agreement with experiment⁶⁾. For the transition $1s \rightarrow 2s$ in H the agreement is much less good³⁾, but (2) still gives cross sections more in accordance with experiment than the Born approximation gives.

Note. For transitions in atomic hydrogen between states with principal quantum numbers $n = 2$ and 3, and between states with principal quantum numbers $n = 3$ and 4, the cross sections for optically allowed excitation increase¹⁾ with increasing azimuthal quantum number l of the initial state, while the cross sections for optically disallowed excitation decrease with increasing l . For ionization the situation is just the opposite¹⁾; for ionization from initial states with $n = 2$ or 3, the cross sections for optically allowed transitions are largest for small l and the cross sections for optically disallowed transitions are largest for large l . In this sense, allowed and disallowed processes are competitive for these transitions. Ionization and excitation are also competitive; this also follows from the sum rules for the oscillator strengths⁷⁾ and the generalized oscillator strengths⁸⁾. It is questionable if this competitive behaviour is fully valid near threshold.

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