ON THE CALCULATION OF RADIAL INTEGRALS OF MULTIPOLE TRANSITIONS IN ATOMIC SPECTRA

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Abstract

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ON THE CALCULATION OF RADIAL INTEGRALS OF MULTIPOLE TRANSITIONS IN ATOMIC SPECTRA

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To calculate the probabilities of multipole radiation and excitation, it is necessary to know the radial integrals

$$R_\chi = \int_0^\infty P_{n_1 l_1} r^\chi P_{n_2 l_2}\, dr, \tag{1}$$

where $P_{n_1 l_1}$ and $P_{n_2 l_2}$ are the radial parts of the wave functions of the initial and final states; χ is the multipolarity of the transition. Bates and Damgaard developed a semiempirical method that makes it possible to calculate radial integrals for dipole transitions ([1]). This method can be extended to the case of arbitrary multipolarity χ. For this purpose we shall consider the essence of the Bates–Damgaard method.

The radial wave functions are written in Coulomb form

$$P_{n^* l}(\rho) = \sqrt{Z}\, K_{n^*, l} W_{n^*, l+1/2}(2\rho/n^*), \tag{2}$$

where $\rho = Zr$; Z is the charge of the atomic core; $W_{n^*, l+1/2}$ is the Whittaker function; n^* is the effective principal quantum number, determined by the expression $E_{n^*} = Z^2/n^{*2}$, where E_{n^*} is the experimental value of the ionization energy from the given state, expressed in units of $Ry = 13.6$ eV;

$$K_{n^* l} = [\xi_{n^*} n^* \Gamma(n^* + l + 1)\Gamma(n^* - l)]^{-1/2}$$

is the normalization factor. Here

$$\xi_{n^*} = 1 + (2/n^*)\, \partial\mu(E_{n^*})/\partial E_{n^*},$$

where $\mu(E_{n^*}) = n - n^*$ is the quantum defect. Bates and Damgaard assume $\mu = \text{const}$ and, consequently, $\xi = 1$. In reality this is valid only for sufficiently high levels. For lower levels $\mu \neq \text{const}$. Seaton showed ([2]) that for configurations of the type $2p^n$

$$\xi_{n^*} = (n^* - 1)(n^* + 2)/[n^*(n^* + 1)].$$

If the asymptotic expansion of the Whittaker function is used, expression (2) takes the form

$$P_{n^*l} = \sqrt{Z} K_{n^*l} \left(\frac{2\rho}{n^*}\right)^{n^*} e^{-\rho/n^*} \sum_{t=0}^{\infty} b_t \rho^{-t}, \tag{3}$$

where

$$b_0 = 1, \qquad b_t = \frac{n^*}{2t} \left[l(l+1) - (n^* - t)(n^* - t + 1)\right] b_{t-1}.$$

The summation may be restricted to the term with index $n^* + l - 1 < t_0 < n^* + l$. The subsequent terms of the expansion in our calculations gave a contribution of less than 1%.

Now, substituting the radial functions (3) into formula (1) and carrying out the integration, we obtain

$$R_\chi = Z^{-\chi} K_{n_1^* l_1} K_{n_2^* l_2} 2^n \frac{n_1^{*n_1^*} n_2^{*n_2^*}}{n^n} \left(\frac{n_1^* n_2^*}{n}\right)^{\chi+1} \Gamma(n + \chi + 1) \times$$

$$\times \left[1 + \sum_{k=1}^{t_{01}+t_{02}} \left(\frac{n}{n_1^* n_2^*}\right)^k \left[\sum_{t_1+t_2=k} b_{t_1} b_{t_2}\right] \Big/ \left[\prod_{i=0}^{k-1} (n + \varkappa - i)\right]\right], \tag{4}$$

where $n = n_1^* + n_2^*$. Formula (4) makes it possible to calculate transition probabilities for arbitrary multipolarity $\varkappa$. As the order of the multipolarity increases, the accuracy of the method should increase, since with increasing $\varkappa$ the contribution determined by the asymptotics of the radial functions increases (see formula (1)); with increasing r these functions approach the Coulomb functions.

In the particular case $\varkappa = 1$, calculations by formula (4) lead to the results presented in the tables of Bates–Damgaard.

Table 1

Maximum electron-impact excitation cross sections for hydrogen and helium atoms
$\sigma_{\max}/\pi a_0^2$ ($\pi a_0^2 = 8.7 \cdot 10^{-17}$ cm^2)

Element	Transition	This work	Other sources: theory	Other sources: experiment
H	$1s$—$2s$	0.27	0.25 ([4]), 0.73 ([4]), 0.13 ([5])	0.16 ([5])
H	$1s$—$3d$	0.022	0.022 ([4]), 0.025 ([6])	–
He	1^1S—2^1S	0.036	0.017 ([6])	0.028 ([6]), 0.020 ([7])
He	1^1S—4^1S	0.0015	–	0.0024 ([7])
He	1^1S—3^1D	0.0027	0.00082 ([6])	0.0045 ([7])
He	1^1S—4^1D	0.0013	0.00063 ([6])	0.0018 ([7]), 0.00042 ([6])

Table 1 gives the results of calculating the maximum cross sections of quadrupole excitation (3) for several transitions in hydrogen and helium atoms. Alongside the calculations by formula (4), data of other authors are given.

Table 2

Ratio of probabilities of quadrupole and dipole transitions for alkali metals

$$\frac{A_{\text{quad}}}{A_{\text{dip}}} \cdot 10^6$$

Element	This work	Other sources ([8]): theory	Other sources ([8]): experiment
Na	2.8	1.1	3.5
K	2.5	1.5	2.5
Rb	2.0	2.7	2.9
Cs	0.7	0.6	–

Table 3

Transition probabilities for several nebular and auroral lines (in sec^{-1})

Transition	This work	Other sources: theory ([9])	Other sources: experiment ([10])
N II: $2p^2\ \ ^1S$—^1D	1.1	1.3	–
O II: $2p^3\ \ ^2D^\circ_{5/2}$—$^2P^\circ_{3/2}$	0.26	0.24	–

Transition	This work	Other sources: theory ([9])	Other sources: experiment ([10])
O I: $2p^4 \quad {}^1S—{}^1D$	1.2	1.7	1.4±

Table 2 gives the ratios of the probabilities of transitions from the first D-term to the ground state (A_{quad}) to the probabilities of resonance transitions (A_{dip}) for alkali metals. As was to be expected, in the case of radiative transitions better agreement with experiment is observed than in the case of electron-impact excitation. In Table 3 we give the results of calculations of the probabilities of several quadrupole transitions of interest for astrophysics.

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Note: Figure translations are in progress. See original paper for figures.