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The scattering of slow electrons by lithium atoms; improved cross section estimates for transitions between states with $n = 3$

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Abstract. The previously published five-state close-coupling total cross sections of Moores are considered with an improved estimate of the contribution from partial cross sections corresponding to large values of the total angular momentum using the unitarised Bethe approximation and Burgess sum rule method as given by Whelan. Results are presented for transitions between the 3s, 3p and 3d states of a range of energies.

In a recent paper, Moores (1986) presented results for the total cross section for electron impact excitation of atomic lithium. Close coupling in the form of the IMPACT computer program (Crees *et al* 1978) was used to calculate the partial cross sections corresponding to small values of the total angular momentum, while the contribution from the higher L values was estimated by extrapolating in a geometric progression for the diagonal elements of the reactance matrix and by using the Bethe approximation for the off-diagonal elements. Difficulties were encountered in the generation of the Bethe matrix elements with sufficient speed and accuracy to allow converged cross sections to be calculated in all cases. We have made use of the analysis of the Bethe approximation to the reactance matrix given in Whelan (1986) in order to produce converged cross sections for all the transitions considered in the original paper. No attempt has been made to improve on the close-coupling calculations for the lower values of L.

For a 2λ-pole transition from an initial atomic state nl_a to a final state $n'l'_a$ the Bethe approximation to the reactance matrix is proportional to

$$I_0(k, l, k', l', \lambda) = (kk')^{1/2} \int_0^\infty j_l(kr) j_{l'}(k'r) r^{-(\lambda+1)} \, dr \tag{1}$$

where k, l, k' and l' denote the wavenumber and orbital angular momentum of the free electron before and after the collision, respectively, and j_l and $j_{l'}$ are spherical Bessel functions. It should be noted that for $\lambda = 0$ the constant of proportionality, and hence the Bethe matrix element, are both zero.

The major difficulties encountered with the calculation of the Bethe terms come from the evaluation of the Weber-Schafheitlin integral $I_0(k, l, k', l', \lambda)$ when $k \neq k'$.

Whelan (1986) has proved that it may be written:

$$I_0(k, l, k', l', \lambda) = \left(\frac{\pi}{kk'}\right)^{1/2} \frac{1}{2^\lambda \Gamma(\lambda + \frac{1}{2})} \sum_{\mathscr{L}} \mathscr{Q}_{\lambda\mathscr{L}}(k, l, k', l') Q_{\mathscr{L}}(\chi) \tag{2}$$

where $\mathscr{Q}_{\lambda\mathscr{L}}(k, l, k', l')$ is defined in Seaton (1961) and $Q_{\mathscr{L}}(\chi)$ is a Legendre polynomial

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of the second kind whose argument is given by

$$\chi = (k^2 + k'^2)/2kk'. \tag{3}$$

Using this result it is possible to generate large numbers of Bethe reactance matrix elements to a high degree of accuracy and at a very small cost in computer time. Furthermore, in the same paper Whelan showed, following Burgess (1974), that for $\lambda = 1$ and $k = k'$ the weak-coupling Bethe approximation could be summed exactly from $l = l_0$ to infinity and that the sum was proportional to

$$\tfrac{1}{4} l_0 (k/k')(Q^2_{l_0-1}(\chi) - Q^2_{l_0}(\chi)). \tag{4}$$

When $k = k'$, $\lambda \geqslant 1$ the Weber-Schafheitlin integral $I_0(k, l, k', l', \lambda)$ can also be put in a form which is particularly simple to compute reliably (see Watson (1944) and also Whelan (1986)).

We used the five-state close-coupling results as discussed in Moores (1986) for all partial cross sections corresponding to $L \leqslant L_1$, the Bethe approximation to the reactance matrix as discussed above to calculate cross sections for $L_1 < L \leqslant L_2$ and the Burgess sum rules to calculate the contribution from $L = L_2 + 1$ to infinity for the dipole transitions in the weak-coupling Bethe approximation. The values of L_1 and L_2 used are given in table 1. It should be noted that at $L = L_2$ there was no significant difference between the weak- and strong-coupling Bethe approximations. We did not find it necessary to make use of the geometric series for the diagonal elements of the reactance matrix since their neglect had only a negligible effect on the partial cross sections corresponding to the inelastic transitions; indeed after unitarisation even the diagonal elements of the transmission matrices agreed to a very high degree of accuracy.

Table 1. Values of L_1 and L_2. Parity π_1 refers to the coupled channels (2s, L), (2p, $L \pm 1$), (3s, L), (3p, $L \pm 1$), (3d, L, $L \pm 2$) and parity π_2 to the channels (2p, L), (3p, L), (3d, $L \pm 1$).

	π_1		π_2	
k_1^2 (Ryd)	L_1	L_2	L_1	L_2
0.3	15	74	17	73
0.3675	18	74	21	74
$\geqslant$0.45	22	74	21	74

Table 2. Total cross sections in πa_0^2. Numbers in brackets denote multiplication by powers of ten.

k_1^2 (Ryd)	3s→3s	3s→3p	3s→3d	3p→3p	3p→3d	3d→3d
0.3	1068	86	195	4.9 (+3)	7.2 (+3)	7.1 (+3)
0.3675	658	206	259	1.3 (+3)	3.8 (+3)	1.3 (+3)
0.45	480	401	202	7.2 (+2)	2.6 (+3)	6.3 (+2)
0.5	411	464	178	5.7 (+2)	2.2 (+3)	4.9 (+2)
0.55	350	508	166	4.8 (+2)	1.9 (+3)	4.1 (+2)
0.6	319	519	143	4.1 (+2)	1.7 (+3)	3.5 (+2)
0.65	280	531	130	3.6 (+2)	1.6 (+3)	3.1 (+2)
0.7	245	538	130	3.2 (+2)	1.4 (+3)	2.8 (+2)
0.75	228	521	108	2.8 (+2)	1.3 (+3)	2.5 (+2)

We found no significant difference between the results of Moores (1986) and those presented here for transitions from 2s and 2p, but for transitions from states with principal quantum number $n = 3$ there were large differences.

This was particularly true for the dipole transitions $3s \rightarrow 3p$ and $3p \rightarrow 3d$, where a combination of the neglect of contributions from $L > L_2$ and inaccuracies due to difficulties in evaluating the Bethe elements lead to errors of as much as 40%.

We present a full set of results in table 2 for transitions between the sublevels with principal quantum number $n = 3$.

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