

## Theory of anisotropy transfer and calculations of alignment of $np$ states populated in electron capture by highly charged ions

C. D. Lin\*

*Argonne National Laboratory, Argonne, Illinois 60439*

J. H. Macek

*Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588-0111*

(Received 19 January 1987)

The excited states of highly charged ions populated by charge transfer are frequently aligned. The alignment of each  $nl$  level often reflects the initial alignment due to the collision as well as the alignment of higher levels which cascade down to this level. We adapt the theory of alignment transfer and apply it to analyze the alignment of Lyman radiations following ion-atom collisions. The theory is illustrated using computed alignments of higher levels reported earlier and the results are compared with recent measurements.

### I. INTRODUCTION

The wide availability of beams of highly stripped heavy ions has prompted the study of how such ions interact with matter. One of the most probable reactions is the capture of electrons by highly charged ions.<sup>1</sup> Such reactions are of considerable interest, but are difficult to study in detail, both experimentally and theoretically, owing to the large number of Rydberg states populated by capture. On the experimental side, the population of different  $n$  levels or  $nl$  sublevels has been measured by translational energy spectroscopy<sup>2</sup> or by photon- and electron-emission spectroscopy<sup>3</sup> for some systems, while the most common theoretical methods must first calculate amplitudes for populating specific  $nlm$  eigenstates. Appropriate sums must be performed to obtain  $n$  and/or  $nl$  distributions, and much detailed information about the collision is lost in obtaining the total cross sections. Alternatively, it is clearly impossible to experimentally measure complete  $nlm$  distributions by conventional methods for the manifold of Rydberg states populated by capture with high- $Z$  projectiles, even though such measurements would help uncover the mechanisms which operate to populate Rydberg states in collisions involving highly charged species. For this reason interest attaches to quantities which measure other gross features of nonstationary states populated in collisions, such as their shape and circulation properties. Such properties are characterized by the alignment and orientation parameters of Fano and Macek.<sup>4</sup> These parameters are defined for atomic states of specific  $n$  and  $l$ ; to compare them with experiment it is necessary to average them according to the specific experimental arrangement.

Alignment is commonly measured by observing the polarization of collision-induced radiation. The appropriate averages in this case include sums over all of the cascade contributions. For this purpose the alignment parameter is particularly useful since it has simple transfer properties. In contrast, the commonly employed polarization

parameter is much more cumbersome. In this work we used computed  $nlm$  distributions to obtain alignments of dominant  $nl$  levels in the high-energy region for  $O^{8+} + He$  collisions<sup>5,6</sup> and for  $Ne^{9+} + H_2$  collisions at 4 keV/amu.<sup>7</sup> In the latter case we model the primary collision for the population of  $nlm$  states as identical to the distribution for  $O^{8+} + H$  at the same velocity. We then illustrate, using standard alignment transfer theory, how the  $np$  ( $n \geq 2$ ) levels are populated and aligned by cascades from higher levels. General expressions for alignment transfer are given in Sec. II. Using calculated  $nl$  cross sections and initial alignments, in Sec. III we illustrate the calculation of alignments of  $np$  levels by cascades from higher excited levels. The calculated alignments and polarizations are then compared with measurements for  $O^{8+} + He$  and  $Ne^{9+} + H_2$ . Agreement between theory and experiment is reasonable for the former system, but large discrepancies exist for the latter. A short summary is given in Sec. IV.

### II. ALIGNMENT TRANSFER IN CASCADES

Anisotropy transfer and perturbation have been treated in the literature.<sup>4,8-10</sup> The object of this paper is to adapt available treatments to the particular case of alignment of  $np$  states populated by electron capture, taking into account both cascade and spin-orbit effects for hydrogenlike ions. We use the calculations of Jain *et al.*<sup>5</sup> to obtain the initial alignment and standard treatments of anisotropy transfer<sup>8,9</sup> to compute cascade contributions.

To compute the anisotropy transfer we take advantage of some simplifications characteristic of hydrogenic ions but often found in other ions. First, one has that the decay widths are much smaller than the fine-structure splitting. This permits one to compute anisotropy transfer between stationary states labeled by  $LSJ$  quantum numbers. Second, we suppose that Russell-Saunders coupling holds. This allows branching ratios for radiative transitions between fine-structure levels in the decay  $n_{i+1}L_{i+1} \rightarrow n_iL_i$

to be treated by standard angular momentum recoupling theory. Branching to different  $nL$  levels requires a knowledge of radial matrix elements and cannot be treated by angular momentum recoupling. For hydrogenic ions the radial matrix elements and transition probabilities are available in standard references.<sup>11</sup> We therefore compute the anisotropy transfer for each sequence of transitions  $n_N L_N S J_N \rightarrow n_{N-1} L_{N-1} S J_{N-1} \rightarrow \cdots \rightarrow n_1 L_1 S J_1$ . We suppose that the alignment is measured by observing the angular distribution or polarization of radiation emitted in the transitions  $n_1 L_1 S J_1 \rightarrow n_0 L_0 S J_0$ . In this last transition it is usually true that fine structure is not resolved so that it is necessary to sum or average over fine-structure levels  $J_1$  and  $J_0$ . In addition it is necessary to sum over all intermediate fine-structure levels  $J_i$  allowed by dipole selection rules. This gives the anisotropy transfer factor for the chain  $n_N L_N \rightarrow n_{N-1} L_{N-1} \rightarrow \cdots \rightarrow n_1 L_1$ . When several such chains contribute to the population of level 1, then it is necessary to average over the contribution from each chain weighted according to the branching ratios for the various intermediate  $n_i L_i$  levels and the initial population of level  $N$ . Our purpose here is to compute the transfer factor for a given chain. These factors are then used in Sec. III to compute the alignment of  $np$  levels of hydrogenic ions populated by electron capture, taking into

account cascade contributions from all possible cascade chains.

To carry out this task we use standard results on anisotropy transfer theory.<sup>8</sup> Let  ${}^{J_i} \sigma_q^k$  denote the unnormalized  $kq$ th-state multipole<sup>12</sup> of the level  $J_i$ :

$${}^{J_i} \sigma_q^k = \sum_{m, m'} \sigma_{mm'}(J_i m J_i - m' | k q) (-1)^{J_i - m'} . \quad (1)$$

This multipole is represented by the coupling scheme  $(J_i J_i)k$ . If  $J_i$  is populated by cascade transitions from  $J_{i+1}$ , the  $k$ th multipole of the upper level is represented by the coupling scheme  $(J_{i+1} J_{i+1})k$ . The dipole transition matrix is represented by the coupling scheme  $(J_i J_{i+1})1$ . The states are coupled by radiative transitions characterized by the dipole transition operator  $(\hat{\epsilon}^\dagger \cdot \mathbf{r})(\hat{\epsilon} \cdot \mathbf{r}')$  averaged over directions and polarizations of the photon

$$\overline{(\hat{\epsilon}^\dagger \cdot \mathbf{r})(\hat{\epsilon} \cdot \mathbf{r}')} = \mathbf{r} \cdot \mathbf{r}' / 3 . \quad (2)$$

Since this operator is a scalar, the average squared dipole matrix element is characterized by the coupling scheme  $(J_i J_{i+1})1(J_i J_{i+1})1, 0$ . The alignment transfer factor just represents a recoupling of  $(J_i J_i)k(J_{i+1} J_{i+1})k', 0$  to yield the coupling  $(J_i J_{i+1})1(J_i J_{i+1})1, 0$ . A detailed treatment<sup>8</sup> gives

$${}^{J_i} \sigma_q^k = C'(J_{i+1} || r || J_i)^2 (2k+1)^{-1/2} 3^{-1/2} \sum_k ((J_{i+1} J_i)1(J_i J_{i+1})1 | (J_i J_i)k(J_{i+1} J_{i+1})k')^{(0) J_{i+1}} \sigma_q^{k'} , \quad (3)$$

where  $C'$  is a constant independent of  $J_{i+1}$ ,  $J_i$ , and  $k$ . Because  $kk'$  couple to 0, terms with  $k \neq k'$  vanish in the sum over  $k'$ . This follows from the general theorem that scalar interactions, represented in this case by the operator in Eq. (2), cannot change the rank of a state multipole.<sup>12</sup> Note that the state multipoles are not normalized. Since many intermediate levels are possible in cascade transitions, it is convenient to defer normalization until the alignment for the levels  $(SL_1)J_1$  populated by a single chain of cascade transitions has been obtained. Reduced matrix elements in Eq. (3) and throughout this work are defined according to Eq. (5.4.1) of the book by Edmonds.<sup>13</sup>

In order to sum over both  $J_i$  and  $J_{i+1}$  it is necessary to extract the  $J$  dependence of the reduced matrix element explicitly. In a more complete notation we have

$$\begin{aligned} & (L_{i+1} S J_{i+1} || r || L_i S J_i)^2 \\ &= (L_{i+1} || r || L_i)^2 (2J_{i+1} + 1)(2J_i + 1) \\ & \quad \times \begin{Bmatrix} L_{i+1} & J_{i+1} & S \\ J_i & L_i & 1 \end{Bmatrix}^2 . \end{aligned} \quad (4)$$

Defining  $C_i = C'(L_{i+1} || r || L_i)^2$  and using Eq. (4) in Eq. (3) with the recoupling coefficient written in terms of 6- $J$  symbols, we have the result

$${}^{J_i} \sigma_q^k = C_i B(k, J_i J_{i+1})^{J_{i+1}} \sigma_q^k , \quad (5)$$

where

$$\begin{aligned} & B(k, J_i J_{i+1}) \\ &= (2J_{i+1} + 1)(2J_i + 1) (-1)^{J_{i+1} + J_i + 1 + k} \\ & \quad \times \begin{Bmatrix} L_{i+1} & J_{i+1} & S \\ J_i & L_i & 1 \end{Bmatrix}^2 \begin{Bmatrix} J_{i+1} & J_i & 1 \\ J_i & J_{i+1} & k \end{Bmatrix} . \end{aligned} \quad (6)$$

Equations (5) and (6) give the anisotropy transfer for the transition  $J_{i+1} \rightarrow J_i$ . The anisotropy of the level  $L_1 S J_1$  of interest involves many sequences of such binary alignment transfers. The alignment of level 1 is computed by summing over all such transfers. We therefore have

$${}^{J_1} \sigma_q^k = \prod_i C_i \sum_{J_N} D(k, J_1 J_N)^{J_N} \sigma_q^k , \quad (7)$$

where

$$D(k, J_1 J_N) = \sum_{J_2, J_3, \dots, J_{N-1}} B(k, J_1 J_2) B(k, J_2 J_3) \cdots B(k, J_{N-1} J_N), \quad N > 2$$

$$D(k, J_1 J_N) = B(k, J_1 J_2), \quad N = 2 \quad (8)$$

$$D(k, J_1 J_N) = \delta(J_1 J_N), \quad N = 1 .$$

The factors  $C_i$  are unimportant for our present purposes since they will divide out when the state multipoles for level 1 are normalized. These factors just represent the branching ratios for the level  $n_{i+1}L_{i+1}$  to populate the level  $n_iL_i$ . If several different cascade chains populate level 1, then these factors must be incorporated into the averaging over alternative paths to determine the aver-

age alignment of level 1.

The alignment transfer factor relates to the transfer from a  $J_N$  level which is part of a fine-structure multiplet. To relate this to the initial alignment formed by electron capture, we employ the hypothesis of Percival and Seaton,<sup>14</sup> namely,

$$J_N \sigma_q^k = (-1)^{-S-L_N-J_N+k} \frac{(2J_N+1)}{(2S+1)} \begin{Bmatrix} L_N & L_N & k \\ J_N & J_N & S \end{Bmatrix} L_N \sigma_q^k. \quad (9)$$

The Fano-Macek<sup>4</sup> anisotropy parameters are given in terms of expectation values of nonstandard irreducible tensors  $T_q^{[k]}$  constructed from angular momentum operators. When  $LS$  coupling holds to a good approximation, then the relevant operators are constructed from orbital angular momentum operators  $L$ . In particular the single nonvanishing component of the alignment tensor is proportional to the expectation value of  $3L_z^2 - L^2$ . These expectation values are denoted by  $\langle (L | T_q^{[k]} | L) \rangle$  and are normalized by dividing by  $\langle (L | T_0^{[0]} | L) \rangle$ .

Using the definition of the state multipoles and the Wigner-Eckart theorem, we have

$$\begin{aligned} \langle (L_1 | T_q^{[k]} | L_1) \rangle &= \sum_{J_1} \langle (J_1 | T_q^{[k]} | J_1) \rangle \\ &= (2k+1)^{-1/2} (L_1 || T^{[k]} || L_1) \sum_{J_1} (-1)^{S+L_1+J_1+k} (2J_1+1) \begin{Bmatrix} L_1 & J_1 & S \\ J_1 & L_1 & k \end{Bmatrix} J_1 \sigma_q^k. \end{aligned} \quad (10)$$

Equation (10) together with Eqs. (7), (8), and (9) give the expectation values of irreducible tensors in terms of the state multipoles of level  $N$ . These expectation values are normalized by dividing by the mean value of the zeroth rank tensor. This ratio for level  $N$  is just given by

$$\langle (L_N | T_q^k | L_N) \rangle / \langle (L_N | T_0^0 | L_N) \rangle = (2k+1)^{-1/2} [(L_N || T^{[k]} || L_N) / (L_N || T^{[0]} || L_N)] (L_N \sigma_q^k / L_N \sigma_0^0). \quad (11)$$

Substituting Eqs. (9), (10), and (11) into Eq. (7), we obtain the anisotropy parameters from level 1 populated by cascade transitions from level  $N$  in terms of the anisotropy of level  $N$ :

$$\begin{aligned} \frac{\langle (L_1 | T_q^{[k]} | L_1) \rangle}{\langle (L_1 | T_0^{[0]} | L_1) \rangle} &= \frac{(L_1 || T^{[k]} || L_1) (L_N || T^{[0]} || L_N)}{(L_1 || T^{[0]} || L_1) (L_N || T^{[k]} || L_N)} \\ &\times \left[ \sum_{J_1, J_N} (-1)^{L_1-L_N+J_1-J_N} \frac{(2J_1+1)(2J_N+1)}{(2S+1)} \begin{Bmatrix} L_1 & J_1 & S \\ J_1 & L_1 & k \end{Bmatrix} D(k, J_1 J_N) \begin{Bmatrix} L_N & J_N & S \\ J_N & L_N & k \end{Bmatrix} \right] \\ &\times \left[ \sum_{J_1, J_N} (-1)^{L_1-L_N+J_1-J_N} \frac{(2J_1+1)(2J_N+1)}{(2S+1)} \begin{Bmatrix} L_1 & J_1 & S \\ J_1 & L_1 & 0 \end{Bmatrix} D(0, J_1 J_N) \right. \\ &\quad \left. \times \begin{Bmatrix} L_N & J_N & S \\ J_N & L_N & 0 \end{Bmatrix} \right]^{-1} \frac{\langle (L_N | T_q^{[k]} | L_N) \rangle}{\langle (L_N | T_0^{[0]} | L_N) \rangle}, \end{aligned} \quad (12)$$

where  $D(k, J_1 J_N)$  is given by Eqs. (6) and (8).

The second factor in large parentheses is evaluated directly to obtain

$$\begin{aligned} &\left[ \sum_{J_1, J_N} (-1)^{L_1-L_N+J_1-J_N} \frac{(2J_1+1)(2J_N+1)}{(2S+1)} D(0, J_1 J_N) \begin{Bmatrix} L_N & J_N & S \\ J_N & L_N & 0 \end{Bmatrix} \right]^{-1} \\ &= (2L_1+1)^{1/2} (2L_2+1)(2L_3+1) \cdots (2L_{N-1}+1)(2L_N+1)^{1/2}. \end{aligned} \quad (13)$$

Equation (13) serves as a check on computer programs used to compute the first term in large parentheses for arbitrary  $k$ .

We have obtained the transfer for arbitrary rank tensors; however, the alignment parameter in the collision frame  $A_0^{\text{col}}(L_1)$  corresponding to  $k=2$  and  $q=0$  is of most interest. In this case we use  $T_0^{[2]} = 3L_z^2 - L^2$  and  $T_0^{[0]} = L^2$ . Expli-

cit evaluation of the reduced matrix elements gives

$$\begin{aligned}
 A_0^{\text{col}}(L_1) &= \zeta A_0^{\text{col}}(L_N) \\
 &= \left[ \frac{(L_1 + \frac{3}{2})(L_1 - \frac{1}{2})}{L_1(L_1 + 1)} \frac{L_N(L_N + 1)}{(L_N + \frac{3}{2})(L_N - \frac{1}{2})} \right]^{1/2} \\
 &\times \left[ \sum_{J_1, J_N} (-1)^{L_1 - J_N + J_1 - J_N} \frac{(2J_1 + 1)(2J_N + 1)}{(2S + 1)} \begin{Bmatrix} L_1 & J_1 & S \\ J_1 & L_1 & k \end{Bmatrix} D(k, J_1 J_N) \begin{Bmatrix} L_N & J_N & S \\ J_N & L_N & k \end{Bmatrix} \right] \\
 &\times (2L_1 + 1)^{1/2} (2L_2 + 1) \cdots (2L_{N-1} + 1) (2L_N + 1)^{1/2} A_0^{\text{col}}(L_N), \tag{14}
 \end{aligned}$$

with  $k = 2$ .

Equation (14) defines the alignment transfer factor  $\zeta$ , although, strictly speaking, the factor  $\zeta$  includes both alignment transfer proper and dealignment due to spin-orbit interactions. Throughout this work we refer to  $\zeta$  as an alignment transfer factor even though it differs from unity for  $N = 1$  owing to spin-orbit interactions.

This formula is used in Sec. III to evaluate the alignment of  $np$  levels of hydrogenic ions populated by electron capture using the data of Ref. 5. Useful checks on these formulas are provided by evaluating various special cases that can be obtained by more elementary methods.

Consider the case where level 1 and level  $N$  are identical, i.e., there is no cascade transition. Then the factor  $D(k, J_1 J_N)$  is replaced by  $\delta(J_1 J_N)$  and one has  $N = 1$  in

Eq. (12). The resulting equation just relates the initial alignment of level 1 to the alignment pertinent to observations which average over the fine-structure oscillations<sup>15</sup> to give the averaged perturbation factor<sup>10</sup>  $\overline{G(L)}_k$ :

$$\overline{G(L)}_k = \sum_J \frac{(2J + 1)^2}{(2S + 1)} \begin{Bmatrix} L & J & S \\ J & L & k \end{Bmatrix}^2. \tag{15}$$

Equation (15) just represents the effect of spin-orbit interactions in the absence of cascades. Alternatively, consider cascades in the absence of fine structure, that is, when  $S = 0$ . For simplicity consider that level 1 is populated by cascades from level 2 with  $L_2 = L_1 + 1$ . Explicit evaluation of the 6- $j$  symbols in Eq. (14) gives the simple result

TABLE I. Alignment transfer coefficients due to cascades and spin-orbit interactions for (a)  $S = \frac{1}{2}$  and (b)  $S = 1$  states. The initial angular momentum of the excited state  $L_N$  is listed in the first row; the final angular momentum  $L_1$  of the excited state is listed as the first column. Only dipole transitions where the angular momentum decreases by one unit in each step are considered. For example, if  $L_N = 4$ ,  $L_1 = 1$ , the considered cascade is  $4 \rightarrow 3 \rightarrow 2 \rightarrow 1$ . The diagonal elements reflect the average over spin-orbit interactions.

$L_N \backslash L_1$	1	2	3	4	5	6	7	8	9
(a) $S = \frac{1}{2}$									
9									0.983 38
8								0.979 24	0.961 96
7							0.973 33	0.951 70	0.934 91
6						0.964 50	0.936 67	0.915 86	0.899 71
5					0.950 41	0.913 37	0.887 05	0.867 37	0.852 08
4				0.925 93	0.874 84	0.840 48	0.816 31	0.798 23	0.784 18
3			0.877 55	0.802 42	0.758 11	0.728 77	0.707 63	0.692 30	0.680 16
2		0.760 00	0.647 18	0.592 96	0.560 78	0.539 73	0.524 14	0.512 69	0.503 79
1	0.333 33	0.246 67	0.216 93	0.201 50	0.191 50	0.184 73	0.180 01	0.176 35	0.173 46
(b) $S = 1$									
9									0.956 17
8								0.945 41	0.931 85
7							0.930 17	0.913 86	0.900 76
6						0.907 60	0.887 77	0.872 71	0.859 75
5					0.872 23	0.847 97	0.829 50	0.815 02	0.803 38
4				0.812 53	0.783 17	0.761 54	0.745 07	0.731 74	0.721 52
3			0.701 53	0.668 78	0.645 10	0.627 58	0.614 18	0.603 36	0.595 29
2		0.473 33	0.450 16	0.430 67	0.416 45	0.406 00	0.397 75	0.391 24	0.385 94
1	0.277 78	0.150 56	0.133 97	0.126 66	0.122 13	0.118 94	0.116 55	0.114 68	0.113 16

$$A_0^{\text{col}}(L_1) = [(2L_1 - 1)(L_2 + 1)] / [(2L_2 - 1)(L_1 + 1)] \\ \times A_0^{\text{col}}(L_2). \quad (16)$$

The ratio of the alignments of levels 1 and 2 can be computed directly since the ratio is independent of the actual alignment of the initial level. Thus if we suppose that only the levels with  $|M_2| = L_2$  are populated, then these levels can only decay to levels with  $|M_1| = L_1$ . The alignment of a level with only  $|M| = L$  populated is just

$$A_0^{\text{col}}(L) = [3L^2 - L(L + 1)] / L(L + 1) \\ = (2L - 1) / (L + 1) \quad (17)$$

so that the alignment ratio is

$$\zeta = [(2L_1 - 1)(L_2 + 1)] / [(2L_2 - 1)(L_1 + 1)], \quad (18) \\ L_2 = L_1 + 1,$$

in agreement with Eq. (16). Repeated application of Eq. (18) gives

$$A_0^{\text{col}}(L_1) = \frac{2L_1 - 1}{L_1 + 1} \frac{L_N + 1}{2L_N - 1} A_0^{\text{col}}(L_N). \quad (19)$$

For  $p \rightarrow s$  transitions the observed quantity, namely, the polarization of the emitted light  $P$ , is related to the alignment according to

$$P = -3A^{\text{col}} / (2 - A^{\text{col}}). \quad (20)$$

In practical applications, one needs only to consider cascade transitions involving dipole transitions in which each step is  $L \rightarrow L - 1$ . Radiative transitions involving  $L \rightarrow L + 1$  have small branching ratios and can be neglected. For these  $L \rightarrow L - 1$  cascade channels, the alignment transfer coefficients for  $S = 0$  are given by the analytical expression (19). For  $S = \frac{1}{2}$  and  $S = 1$  we tabulate the results for  $L = 2-9$  in Table I. These results are independent of the charge of the ionic species.

### III. ILLUSTRATIVE EXAMPLES

In this section we use the formula developed in Sec. II to calculate the polarization of the emitted radiation by excited atoms. We will consider excited states formed through charge-transfer processes in ion-atom collisions only. From the formulation of Sec. II, we calculate the alignment of the excited state from which the polarization of the emitted radiation is obtained.

The alignment of an excited state  $i$  is determined by the alignment of the state produced in a collision and by the transfer of alignment due to the cascade from the higher states  $j$ . To evaluate the alignment of state  $i$  we need to calculate the weighted alignment from all the possible cascade channels. Let the cross section and the alignment for state  $j$  produced by the collision be  $\sigma_j$  and  $A_0^{\text{col}}(j)$ , respectively. If the fraction of radiative transitions from state  $j$  to state  $i$  via branch  $k$  is  $\omega_k(j)$  and the alignment transfer coefficient is  $\zeta_k(j)$ , the alignment for state  $i$  is given by

$$A_0^{\text{col}}(i) = \frac{\sum_j \sum_k \omega_k(j) [\zeta_k(j) A_0^{\text{col}}(j)] \sigma_j}{\sum_j \sum_k \omega_k(j) \sigma_j}, \quad (21)$$

where the summation is over all the cascade branches  $k$  and states  $j$ . The alignment transfer from each cascade branch is calculated using Eq. (14). In general the summation is truncated assuming contributions from very highly excited states are negligible.

We now use Eq. (21) to calculate the Lyman- $\alpha$  radiation emitted following electron capture in  $\text{O}^{8+}$ -He collisions. This system has been studied theoretically by Jain *et al.*<sup>5</sup> and the results were compared with the polarization data of Ellsworth *et al.*<sup>6</sup> In the analysis of Jain *et al.*, the effects of spin-orbit interactions for the initial and intermediate states of each cascade chain are not correctly included. We provide the proper analysis here using Eq. (21).

We illustrate the calculation of the alignment of the  $2p$  state for  $\text{O}^{8+}$  on He at 5 MeV. The parameters relevant to the calculation are given in Table II. Firstly, the cross section for each  $nl$  state and its alignment are obtained from the *ab initio* calculation using a two-center atomic orbital expansion method. The data used here are taken from Jain *et al.*<sup>5</sup> where capture cross sections to  $n = 2, 3$ , and 4 states of  $\text{O}^{7+}$  were calculated. In Table II only those data relevant to the cascade to  $2p$  are included. The alignment transfer coefficients for each cascade channel are taken from Table I. We also include the  $4p-3d-2p$  cascade to show that contributions involving  $L \rightarrow L + 1$  type transitions are small. Note that the alignment is completely lost for an initial  $s$  state and for chains where  $s$  state is an intermediate state. The fraction of radiative transitions from an initial state  $i$  to the  $2p$  state is evaluated using the table given in Bethe and Salpeter.<sup>11</sup> Note that we also include  $2p$  to  $2p$  "transitions" in the table to account for the effect due to the spin-orbit coupling. From this table it is clear that the dominant contribution to  $2p$  alignment is due to the  $3d-2p$  transition, with substantial contributions from  $4f-3d-2p$  and  $4d-2p$  branches as well. The final alignment of  $-0.157$  is small compared with the initial alignment of each excited state which shows strong alignment (see column 2 of Table II). This significant loss of alignment is due to the cascade effect as well as to spin-orbit interactions. We note from Table II that the alignment transfer coefficient for each cascade branch is only about 0.2, thus reducing the strong alignment of the initially populated excited states.

Using the simple relation between alignment  $A$  and polarization fraction  $P$  for the radiative decay for an  $np$  state,  $P = 3A / (A - 2)$ , the predicted polarization fractions for the Lyman- $\alpha$  radiation resulting from  $\text{O}^{8+}$  on He collisions are shown in Fig. 1 in the energy range 5-36 MeV. The only experimental data<sup>6</sup> point is at 16 MeV where the measured value is  $(17.6 \pm 3)\%$ , while the calculated value is 22.8%. The small discrepancy is probably due to the neglect in the calculation of contributions from the cascade of  $n > 4$  excited states. Including these higher states would tend to reduce the polarization.

We next analyze the polarization of Lyman radiations emitted after the collisions of  $\text{Ne}^{9+}$  on  $\text{H}_2$  at 4 keV/amu

TABLE II. Analysis of alignment parameter for the  $2p$  state of  $O^{7+}$  for  $O^{8+}$  on He at 5 MeV.

Channel	$A_0^{\text{col}}(j)^a$	$(\zeta_k)^b$	$(\omega_k)^c$	$(\sigma_j)^a$	$\omega_k \sigma_j$	$\omega_k \sigma_j \zeta_k A_0^{\text{col}}$
$4f \rightarrow 3d \rightarrow 2p$	-0.757	0.217	1	1.21	1.21	-0.199
$4d \rightarrow 2p$	-0.725	0.247	0.744	1.33	0.99	-0.177
$4p \rightarrow 3d \rightarrow 2p$	-0.642	0.168	0.0037	0.49	0.0	0.0
$4p \rightarrow 3s \rightarrow 2p$	-0.642	0	0.037	0.49	0.02	0.0
$4s \rightarrow 2p$	0	0	0.581	0.167	0.07	0.0
$3s \rightarrow 2p$	0	0	1	0.22	0.22	0.0
$3d \rightarrow 2p$	-0.634	0.247	1	2.40	2.40	-0.375
$2p \rightarrow 2p$	-0.230	0.333	1	1.32	1.32	-0.101
				sum =	6.23	-0.85
					$A_0^{\text{col}}(2p) = -0.137$	
					$P = 19.2\%$	

<sup>a</sup>Initial alignment and subshell cross sections from the calculation of Ref. 5;  $\sigma_j$  is in units of  $10^{-17} \text{ cm}^2$ .

<sup>b</sup>Alignment transfer coefficient from Table I and from Eq. (14).

<sup>c</sup>Branching ratio calculated from Ref. 11.

to compare with the measurement of Vernhet *et al.*<sup>7</sup> We model this problem by assuming that the initial  $nlm$  distribution is the same as the collision of  $O^{8+}$  on H at 4 keV/amu. This model is supported by the agreement of the measured  $np$  fraction for a given  $n$  manifold and the measured average angular momentum  $\langle l \rangle$  with the theoretically calculated results for  $O^{8+}$  on H. The partial  $nlm$  cross sections for  $O^{8+}$  on H were taken from the calculation of Fritsch and Lin<sup>16</sup> where an extended coupled channel calculations using two-center atomic orbitals were employed. This calculation obtains the  $nlm$  capture cross sections to the  $n = 4, 5,$  and  $6$  excited states of  $O^{7+}$ .

In the model calculation, we assume that singlet and triplet states are populated equally for each  $nlm$  and that radiations from triplet states are not measured since they decay to the metastable  $1s2s\ ^3S^e$  and  $1s2p\ ^3P^0$  states. The cascade analysis is performed for  $^1P^0$  states, i.e.,  $S=0$ . In this analysis, we include only  $L \rightarrow L-1$  type transitions for each cascade branch. Since  $S=0$ , we can use the analytical expression (19) to evaluate the alignment transfer coefficient. We also assume that the radiative

branching ratios for the heliumlike neon are identical to the corresponding transitions in the hydrogenlike neon. The final results for the polarizations of all the Lyman transitions are listed in Table III. In Table III we also comment on the dominant contributions to the alignment of each  $np$  state. We note that for  $n=5$  and  $6$ , the polarization is entirely due to the collisionally produced  $np$  states, while for  $n=4$ , there are comparable contributions from the collisionally produced  $4p$  state and cascade contribution from the  $5d-4p$  transition. For  $n=3$  and  $2$ , the polarizations are due to cascade contributions.

The agreement between the theoretical results with experimental data in Table III is quite poor. In general, the calculated polarizations are smaller than the experimental ones except for the  $2p-1s$  transition where the experimental result is smaller. (Experimental result for  $2p-1s$  transition includes contribution from the decay of triplet states which is not considered in the present model.) It is not obvious to us that the approximations made in our model can explain the large measured polarizations. At this time we suspect that the large measured polarizations are due

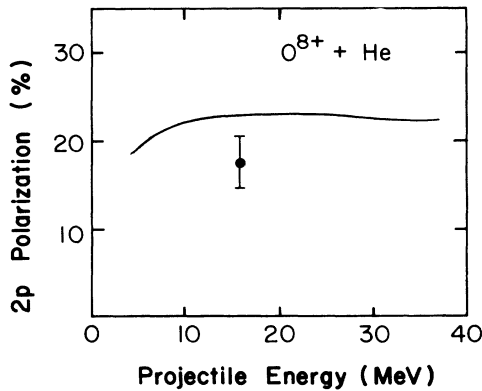


FIG. 1. Polarization fraction of Lyman- $\alpha$  radiation of  $O^{7+}$  following charge transfer in  $O^{8+} + \text{He}$  collisions. Contributions due to cascade from higher channels and effects of spin-orbit interaction are included. The experimental point is from Ref. 6.

TABLE III. Polarization fractions of Lyman x-ray intensities in 4-keV/amu charge-exchange collisions of  $\text{Ne}^{9+} \rightarrow \text{H}_2$ .

	Expt. <sup>a</sup>	Theory <sup>b</sup>	Comments <sup>c</sup>
$6p \rightarrow 1s$	> 58%	41%	Direct <sup>d</sup>
$5p \rightarrow 1s$	$(59 \pm 21)\%$	27%	Direct <sup>d</sup>
$4p \rightarrow 1s$	$(69 \pm 20)\%$	19%	Direct <sup>d</sup> and $5d \rightarrow 4p$
$3p \rightarrow 1s$	$(69 \pm 19)\%$	20%	$5d \rightarrow 3p$ and $5f \rightarrow 4d \rightarrow 3p$
$2p \rightarrow 1s$	$(7 \pm 7)\%$	25%	$5g \rightarrow 4f \rightarrow 3d \rightarrow 2p$ $5f \rightarrow 4d \rightarrow 2p$ $5f \rightarrow 3d \rightarrow 2p$ $5d \rightarrow 2p$ $6h \rightarrow 5g \rightarrow 4f \rightarrow 3d \rightarrow 2p$

<sup>a</sup>Data from Ref. 7.

<sup>b</sup>Calculated for  $O^{8+}-\text{H}$  at the same velocity. Cascade effect is analyzed for  $S=0$ .

<sup>c</sup>Indicates the dominant contributions to the alignment of the  $np$  state.

<sup>d</sup>From direct  $np$  populated in the collision.

to the contribution from double-capture channels. Since the measurement was performed on  $H_2$  targets, a simple estimate suggests that capture to doubly excited states of  $1s5l5l'$  and  $1s4l5l'$  types are likely. The low-lying doubly excited states of  $1s5l5l'$  type are estimated to lie below  $1s4l$  states. Therefore these doubly excited states can autoionize to  $1s3p$  and  $1s4p$  states directly, providing contributions to the measured polarizations for the decay of  $1s3p$  and  $1s4p$  states without the loss of alignment by the cascade effect. We can estimate the relative importance of contributions from single and from double captures. In general, one estimates that double-capture cross section is 15–25% of the single-capture cross section. Because only about 5% (10%) of the single capture eventually reaches the  $1s4p$  ( $1s3p$ ) state, the contribution from double capture to  $1s3p$  and  $1s4p$  could be comparable to the contribution from single capture. Unfortunately we are unable to make a reasonable prediction for the contribution from doubly excited states since it would require the knowledge of capture cross section to each doubly excited state and of the alignment of each state after it autoionizes. On the other hand, our speculation can be tested experimentally by performing the polarization measurements in coincidence with the energy gain of the projectiles after the collision.

#### IV. SUMMARY AND DISCUSSION

In this paper we present the formula for the analysis of alignment transfer of excited states due to cascade contri-

butions. The general expression Eq. (14) allows calculations of alignment transfer from one state to another with spin-orbit coupling effects included. This analysis is essential for the comparison of experimental measured polarizations with theoretical calculations. For  $S=0$  the analysis is simple and an analytical expression Eq. (19) can be used. For  $S=\frac{1}{2}$  and  $S=1$  we present a table for the alignment transfer coefficients for the dominant transitions for  $L \leq 9$ . We applied the formula to calculate the polarizations of Lyman radiations for collisions of  $O^{8+}$  on He from 5 to 36 MeV. The measured polarization at 16 MeV is close to the calculated value at this energy. We have also made a model study for the polarizations of Lyman radiations for  $Ne^{9+}$  on  $H_2$ . The theoretical results are in disagreement with measured values. We suspect that contributions from double-capture channels are responsible for the disagreement and suggest that a coincidence measurement of polarizations with the energy gain of the projectiles for the same collision system be carried out.

#### ACKNOWLEDGMENTS

We thank Dr. A. Jain and Dr. W. Fritsch for providing the  $nlm$  cross sections used in this study. Partial support for this work is provided by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, under Contract No. W-31-109-Eng-38 (C.D.L.) and under No. DE-FG02-85ER13440.A001 (J.M.).

\*Permanent address: Cardwell Hall, Department of Physics, Kansas State University, Manhattan, KS 66506.

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