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Fine-structure effects on resonant transfer excitation cross sections for Li-like-ion collisions with H_2 and He

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We have calculated configuration-mixing *LS*-coupling and intermediate-coupling cross sections for the process of resonant transfer excitation followed by x-ray stabilization in collisions of the Li-like ions S^{13+}, Ca^{17+}, Ti^{19+}, V^{20+}, Ni^{25+}, and Ge^{29+} with H_2 and He. Fine-structure interactions preferentially enhance the *KLL* peak (by up to 35% for S^{13+}) over the *KLn* ($n > L$) peak (+5%), and this largely resolves the discrepancy that exists between theoretical *LS*-coupling calculations and experiment over the relative height of the two peaks for the case of $Ca^{17+}+H_2$.

I. INTRODUCTION

Resonant transfer excitation followed by x-ray stabilization (RTEX) provides an alternative way to study the process of dielectronic recombination (DR) besides merged-beam experiments[1-3] and observations of DR satellites in tokamaks.[4-6] The connection between RTEX and DR was established theoretically by Brandt[7] and by Feagin *et al.*[8] following the experiments on $S^{q+}+\mathrm{Ar}$ collisions by Tanis *et al.*[9,10] Better energy resolution is obtained with H_2 and He than with Ar and, subsequently, there have been a number of RTEX experiments for collisions of Li-like ions with H_2 and He.[11-17] Comparisons with theory are based on the *LS*-coupling calculations by McLaughlin *et al.*[18,19] and show a discrepancy between the relative heights of the low (*KLL*) and high (*KLn*, $n > L$) energy peaks, most noticeably for $Ca^{17+}+H_2$.

We have previously[20] found that core fine-structure interactions can mix *LS*-allowed and *LS*-forbidden autoionizing terms giving access to *LS*-allowed radiative channels and thus enhancing the intermediate coupling DR rate coefficient over the *LS*-coupling result. With this in mind, we use AUTOSTRUCTURE[21,22] to calculate configuration-mixing *LS*-coupling and intermediate coupling (IC) RTEX cross sections for collisions of S^{13+}, Ca^{17+}, Ti^{19+}, V^{20+}, Ni^{25+}, and Ge^{29+} with H_2 and He. In Sec. II we briefly describe the theory behind our calculation; in Sec. III we apply it to Li-like ions; in Sec. IV we present our results for those ion-atom collisions for which experimental results are available, and we conclude in Sec. V.

II. THEORY

Using the impulse approximation,[7,8] the total RTEX cross section $\sigma_x(i;\mathrm{tot})$ for an initial state i may be written in terms of energy-averaged DR cross sections $\bar{\sigma}_d(i;j)$, thus

$$\sigma_x(i;\mathrm{tot})=\sum_j J(Q)\bar{\sigma}_d(i;j)\frac{\Delta E_c}{2I}\left[\frac{MI}{E}\right]^{1/2} . \tag{1}$$

$J(Q)$ is the Compton profile[23] with Q given by

$$Q=\frac{1}{2I}\left[E_c-\frac{Em}{M}\right]\left[\frac{MI}{E}\right]^{1/2} , \tag{2}$$

and E is the projectile-ion energy in the laboratory frame, E_c is the energy required to form the doubly excited state j in the rest frame of the ion, M is the ionic mass, m the electron mass, and I is the ionization potential energy of hydrogen.

The energy-averaged DR cross section for a given initial state i through an intermediate state j is given by

$$\bar{\sigma}_d(i;j)=\frac{(2\pi a_0 I)^2}{E_c\Delta E_c}\frac{w(j)}{2w(i)} \times\frac{\tau_0\sum_k A_r(j\rightarrow k)\sum_l A_a(j\rightarrow i,E_c l)}{\sum_h [A_r(j\rightarrow h)+\sum_l A_a(j\rightarrow h,E_c l]} , \tag{3}$$

where $w(j)$ is the statistical weight of the $(N+1)$-electron doubly excited state, $w(i)$ is the statistical weight of the N-electron initial state, the rates are in units of inverse seconds, and $(2\pi a_0)^2\tau_0=2.6741\times 10^{-32}$ $\mathrm{cm}^2\,\mathrm{sec}$. A_a and A_r may be evaluated in configuration-mixing *LS*-coupling and intermediate-coupling approximation using AUTOSTRUCTURE[21] as detailed in the paper by Badnell and Pindzola.[22]

III. APPLICATION TO Li-LIKE IONS

For $n > 2$ we consider

$$\begin{array}{cccc}
 & & & 1s^2 2snl + h\nu_1 \\
 & & 1s2s^2nl & 1s^2 2pnl + h\nu_2 \\
1s^2 2s + kl_c & \rightleftharpoons & 1s2p^2nl \longrightarrow & 1s^2 2s^2 + h\nu_3 \\
 & & 1s2s2pnl & 1s^2 2p^2 + h\nu_4 \\
 & & & 1s^2 2s2p + h\nu_5 \\
 & & \downarrow & \\
 & & 1s^2nl + kl'_c & \\
 & & 1s^2 2p + kl''_c & \\
 & & 1s2s^2 + kl'''_c &
\end{array} \tag{4}$$

where $l_c, l_c'' = l, l\pm1$, $l_c' = 0,1,2$, and $l_c''' = l\pm1$. For $n=2$ we consider

$$1s^2 2s + kl_c \rightleftharpoons \begin{matrix} 1s2s^2 2p \\ 1s2s2p^2 \end{matrix} \xrightarrow{\quad} \begin{matrix} 1s^2 2s^2 + h\nu_1 \\ 1s^2 2s2p + h\nu_2 \\ 1s^2 2p^2 + h\nu_3 \end{matrix} \qquad (5)$$

$$\downarrow$$

$$1s^2 2p + kl_c'$$

where $l_c = 0,1,2$ and $l_c' = 0,1,2,3$.

The $1s^2 2pnl$ configuration in (4) is unstable against autoionization to $1s^2 2s + kl_c$ for large enough n; when this is so we assume that it no longer contributes to the total RTEX cross section. We sum over nl until $\sigma_x(i;\text{tot})$ has converged. We could also consider $1 \rightarrow 3$, etc., core transitions, but their contributions to $\sigma_x(i;\text{tot})$ should be much smaller than that due to the $1 \rightarrow 2$ core transition considered here, due to the $3 \rightarrow 2$ additional autoionizing channel and should only influence our results at the high-energy tail. The radial functions were evaluated as before[20,22] using scaled Thomas-Fermi-Dirac-Amaldi (TFDA) or Slater-type-orbital (STO) model potentials. We note that we have recently[24] used Hartree-Fock frozen-core orbitals in place of the TFDA for the case of Cl^{7+} and found the change in $\bar{\sigma}_d(i;\text{tot})$ to be less than ±10%.

IV. RESULTS

In Figs. 1–8 we present our *LS*-coupling and IC RTEX cross sections for Li-like ions in collisions with H_2 and He, and compare them with experiment where possible. The energy we plot is that of the projectile ion in the laboratory frame times m/M, see Sec. II. Results for those ion-atom combinations not presented are similar to those for the nearest isoelectronic neighbor and detailed results are available from the author.

The reason for the IC enhancement is that the $1s2s2pnl$ $L=l$ terms are forbidden to autoionize back to the ground in *LS* coupling, but in IC spin-orbit interactions mix them with the $L=l\pm1$ terms which can autoionize back to the ground in *LS* coupling. All terms $L=l$, $l\pm1$ can radiatively stabilize in *LS* coupling. When $A_a^{LS} < A_r^{LS}$, this just redistributes the RTEX cross section, but for $A_a^{LS} > A_r^{LS}$ significant enhancement results. Since $A_r \sim Z^4$ and $A_a \sim Z^0$ and A_r (core) $\sim n^0$ and $A_a \sim n^{-3}$, the effect is largest for lower Z and is greater for the *KLL* peak than the *KLn* ($n > L$). If we go to too low a Z then the spin-orbit interaction is too weak to produce significant mixing and little or no enhancement results.[25] Also, $\sigma_x(i;\text{tot})$ is dominated by capture to $l=1$ and due to the operation of the Pauli exclusion principle, $\frac{7}{15}$ of the $1s2s2p^2$ levels that can radiatively stabilize in *LS* coupling are forbidden to autoionize in *LS* coupling, but only $\frac{1}{3}$ of the $1s2s2pnp$ ($n>2$) are so forbidden.

The above effect shows up strongly in the case of $\text{S}^{13+} + \text{H}_2$ (Fig. 1). The *KLL* IC peak lies 35% above the *LS*-coupling value while the *KLn* ($n > L$) peak is only enhanced by 5%. In the experiment by Tanis *et al.*[12] for $\text{S}^{13+} + \text{He}$ (Fig. 2), the broader energy distribution of He over H_2 does not allow a decision to be made over IC versus *LS* coupling. Both are in good agreement with the experiment, the error bars measuring relative uncertainty while absolute uncertainty of ±20% was claimed.[12] However, in the case of $\text{Ca}^{17+} + \text{H}_2$ (Fig. 3), the experiment of Tanis *et al.*[13] clearly favors the IC result over the *LS* coupling; the difference between theory and experiment over the position of the two peaks is just within experimental uncertainty[19] and occurs again in the $\text{Ca}^{17+} + \text{He}$ (Fig. 4) experiment.[11]

McLaughlin and Hahn[19] have calculated *LS*-coupling results for the experiments in Figs. 2–4 and they show the same qualitative behavior as our *LS*-coupling results, but lie around 15% higher. However, they obtain a similar value (0.87) for the ratio of the *KLL* to *KLn* peaks for $\text{Ca}^{17+} + \text{H}_2$ as in our *LS*-coupling calculation (0.90) while

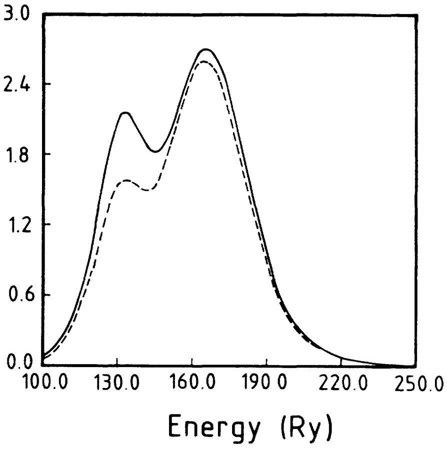

FIG. 1. RTEX cross section for $\text{S}^{13+} + \text{H}_2$. ——, intermediate coupling; — — —, *LS* coupling; both this work.

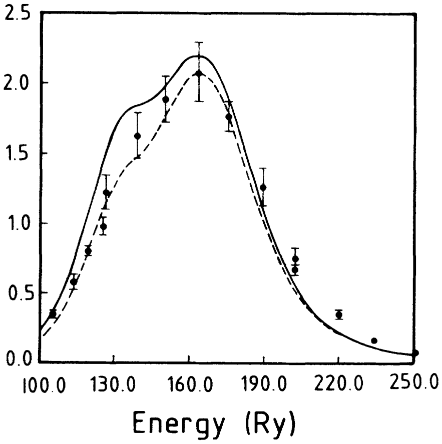

FIG. 2. $\text{S}^{13+} + \text{He}$, as Fig. 1. Dots with error bars are experimental points from Ref. 12.

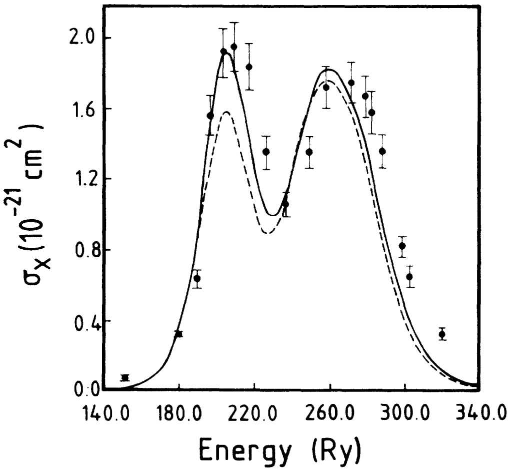

FIG. 3. $Ca^{17+}+H_2$, as Fig. 1. Dots with error bars are experimental points from Ref. 13.

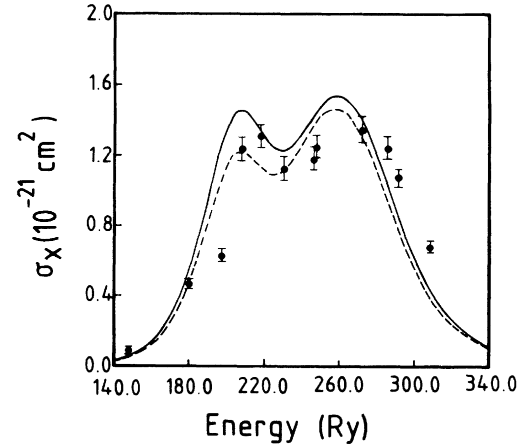

FIG. 4. $Ca^{17+}+He$, as Fig. 1. Dots with error bars are experimental points from Ref. 11.

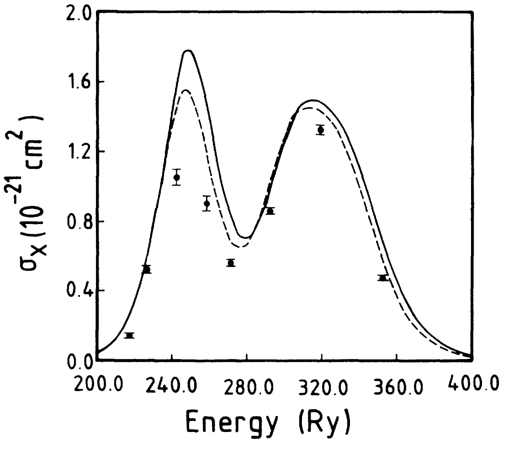

FIG. 5. $Ti^{19+}+H_2$, as Fig. 1. Dots with error bars are experimental points from Ref. 14.

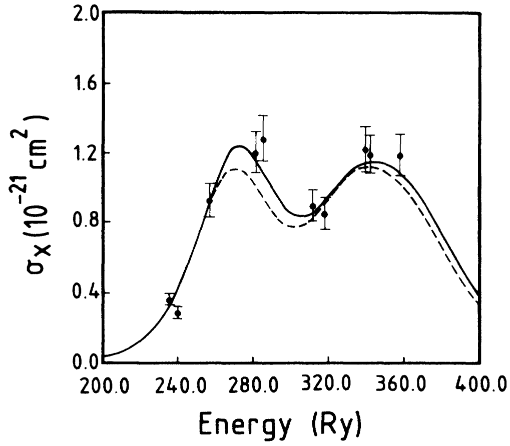

FIG. 6. $V^{20+}+He$, as Fig. 1. Dots with error bars are experimental points from Ref. 11.

in IC we obtain a ratio of 1.05 compared to an experimental value of 1.1 (see Fig. 3). Our ratios remain the same (to within 0.5%) whether we use orbitals generated by STO or TFDA model potentials, although the absolute values of the STO RTEX cross sections, for both *LS* and IC, are about 7% higher than the TFDA. Thus the ratio is much less sensitive to errors in the structure than the absolute cross sections. All the results presented in the figures were obtained using TFDA orbitals.

The IC enhancement of the low-energy peak has dropped to 15% by $Ti^{19+}+H_2$ (Fig. 5), but the IC results are now at slightly higher energies, the position of the resonances being calculated with the Breit-Pauli Hamiltonian as opposed to the nonrelativistic Hamiltonian in the *LS*-coupling case. The experiment of Reusch *et al.*[14] well describes the dip and high-energy peak, but it appears that more experimental data is needed to check out the low-energy peak. Reusch *et al.*[14] also took the theoretical *LS*-coupling results of McLaughlin and

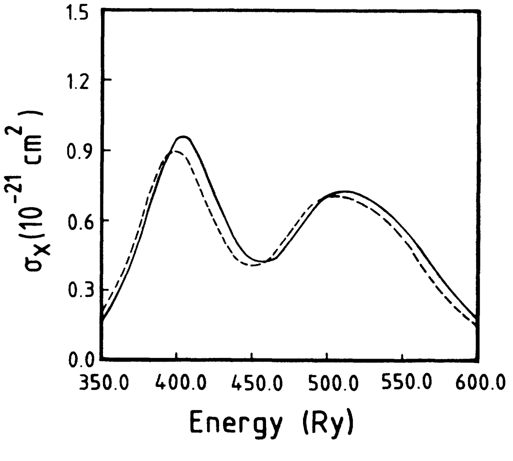

FIG. 7. $Ni^{25+}+He$, as Fig. 1.

Hahn[19] for $Ca^{17+}+H_2$ and scaled them to Ti^{19+} and then normalized to the low-energy peak; not surprisingly, the result[14] they obtained bears no resemblance to our theoretical results. Tanis *et al.*[13] also carried out a normalization of theory to experiment at the low-energy peak for $Ca^{17+}+H_2$ and He. Unfortunately, as we have seen, it is the low-energy nonrelativistic results that are poor, not the high-energy ones.

Both sets of theoretical results are in good agreement with the experiment of Tanis *et al.*[11] for $V^{20+}+He$ (Fig. 6), but the IC results appear to be somewhat better for the low-energy peak. An experiment for $Ni^{25+}+He$ has been carried out by Bernstein *et al.*,[16] but no results have been published yet; our theoretical results are given in Fig. 7. The experiment on $Ge^{29+}+H_2$ (Fig. 8) by Reusch *et al.*[15] reveals a separation of the high-energy peak into *KLM* and *KLn* ($n>M$) components, but our theoretical results (obtained with the Compton profile of Lee[23] for H_2), while showing evidence of the double peak, do not resolve it with the detail obtained by the experiment. The *LS*-coupling results of McLaughlin[15] for $Ge^{29+}+H_2$ are similar to ours.

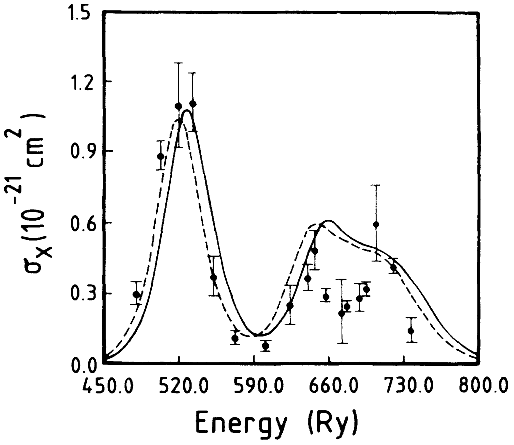

FIG. 8. $Ge^{29+}+H_2$, as Fig. 1. Dots with error bars are experimental points from Ref. 15.

V. CONCLUSION

We have shown that fine-structure interactions enhance RTEX cross sections for Li-like ion collisions with H_2 and He, and preferentially so for *KLL* over *KLn* ($n>L$) peaks. We have shown that this largely resolves the discrepancy between existing theory and experiment over the relative height of the two peaks for $Ca^{17+}+H_2$. Our previous studies[22,24,26] on DR have shown that IC effects are smaller for complex systems than for simpler systems. Consequently, IC effects on RTEX cross sections for *B*-, *C*-like ions, etc., should be much smaller than for Li-like ions. The contribution of $1\rightarrow n$ core transitions ($n>2$) at high energies is currently under investigation.[25]

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