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IMPORTANCE OF CONFIGURATION INTERACTION FOR ACCURATE ATOMIC DATA: FLUORESCENCE YIELDS OF K-SHELL VACANCY, LITHIUM-LIKE IONS

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ABSTRACT

We demonstrate that the inclusion of configuration interaction (CI) results in significant values for the K-shell fluorescence yields of Li-like ions, which are zero in a single-configuration approach. Modeling codes for simulating supernova remnants under nonequilibrium ionization conditions or photoionized plasmas such as active galactic nuclei or X-ray binaries need to be updated accordingly. A two-parameter fitting formula for the fluorescence yields has been developed. The generality of important CI effects on atomic calculations is pointed out.

Subject headings: atomic data — atomic processes — line: formation — X-rays: general

1. INTRODUCTION

Important in both collisionally ionized and X-ray photoionized plasmas is the production of K-shell vacancies in ions, which can decay in a variety of ways with the emission of one or more photons and/or electrons. The probabilities of these competing processes are crucial to the determination of the fundamental characteristics of an astrophysical plasma, notably the ionization balance and the fluorescence and photoabsorption spectra. Clearly, then, insight and understanding of astrophysical plasmas require the availability of accurate atomic data for the rates of the competing radiative and autoionization (Auger) processes. These data are of particular importance for the interpretation of the spectra of photoionized plasmas such as those produced in active galactic nuclei and X-ray binaries (Ferland 2003), as well as for supernova remnants (SNRs) under nonequilibrium ionization conditions. In response to this need, we have embarked upon a calculational program to assess the extant databases for astrophysically relevant fluorescence and Auger yields and to correct any inaccuracies (Gorczyca et al. 2003).

The primary present source of these data is the tables compiled by Kaastra & Mewe (1993), which are based on single-particle central-field atomic calculations for singly ionized atoms, and extrapolation for the remainder of each isoelectronic sequence. These data are used in various astrophysical modeling codes, for example, CLOUDY (Ferland et al. 1998), XSTAR (Kallman & Bautista 2001), and the SNR code of Borkowski et al. (2001). In this Letter, it is pointed out that for certain systems the extant data are completely wrong.

In an earlier publication (Gorczyca et al. 2003), we began to assess the accuracy of the existing, widely used fluorescence and Auger database of Kaastra & Mewe (1993) by focusing on what we initially thought to be the fewest-electron, and therefore simplest, K-shell vacancy system that can fluoresce, namely, the four-electron Be-like $1s2s^22p$ state. Here we show that this is not the case: the three-electron Li-like $1s2s^2$ state does in fact fluoresce once the important many-body interactions (electron correlation, or configuration interaction) are taken into account. Such states are formed either by K-shell ionization of the four-electron Be-like system or by inner shell $1s \rightarrow 2s$ excitation of the three-electron Li-like system.

Before proceeding, we should point out that several works have identified this nonzero fluorescence yield for the Li-like $1s2s^2$ state. For instance, Gabriel (1972) performed intermediate-coupling calculations for a few selected K-shell vacancy Li-like ions, obtaining a fluorescence yield (defined in § 2) for the astrophysically important Fe XXIV ion of roughly 3/10. Later, improved calculations by Chen (1986), who also reported results for only certain selected ions, and more recently Bautista et al. (2003) and Kallman et al. (2004) have modified the Fe XXIV fluorescence yield value to roughly 1/10. However, these two latter works, which also incorporated the data into modeling of ionization balance, were for only one ion (Fe XXIV) in the Li-like isoelectronic sequence. There has also been recent work on the fluorescence yields of oxygen ions (García et al. 2005). However, for Li-like oxygen, only the $1s2p^2$ levels were treated; no data for the $1s2s^2$ level were reported, although we indicate below a way in which the fluorescence yield for this state can be inferred. For all other Li-like ions, to our knowledge, the fluorescence yields in existing databases are zero. The purpose of this Letter is to call attention to such deficiencies in the databases and report new, accurate nonzero values.

2. CALCULATIONAL APPROACH

In the absence of electron correlation, the lowest Li-like K-shell vacancy state can be described exactly by a single-configuration (SC) wave function

$$\Psi^{\rm SC} = 1s2s^2(^2S). \quad (1)$$

Since this wave function contains no *p*-electrons, an ordinary (electric dipole) radiative transition is not possible.[1] Thus, the

[1] Note that a highly forbidden magnetic dipole transition is in fact possible, but the probability is so small that it is essentially ignorable in this situation.

TABLE 1

FLUORESCENCE YIELD ω_K VERSUS NUCLEAR CHARGE Z FOR THE INTERMEDIATE-COUPLING, CI-MIXED Li-LIKE $1s2s^2$ STATES

Z	ω_K^{CI}	ω_K^{fit}	Z	ω_K^{CI}	ω_K^{fit}
4	0.000076	0.000091	18	0.035187	0.034299
5	0.000210	0.000223	19	0.042622	0.041837
6	0.000459	0.000462	20	0.050939	0.050354
7	0.000874	0.000854	21	0.060142	0.059855
8	0.001512	0.001453	22	0.070221	0.070327
9	0.002437	0.002322	23	0.081161	0.081733
10	0.003718	0.003526	24	0.092939	0.094012
11	0.005427	0.005138	25	0.105530	0.107081
12	0.007640	0.007235	26	0.118905	0.120832
13	0.010427	0.009897	27	0.133037	0.135136
14	0.013859	0.013201	28	0.147898	0.149844
15	0.018000	0.017224	29	0.163462	0.164787
16	0.022906	0.022041	30	0.179705	0.179781
17	0.028623	0.027714			

K-shell fluorescence yield ω_K, defined as the probability that the K-shell vacancy will decay radiatively (as opposed to Auger decay), is identically zero, that is,

$$\omega_K^{SC} = 0. \tag{2}$$

Indeed, the tabulated results of Kaastra & Mewe (1993) give a value of zero for every Li-like ion.

However, considering many-body interactions in the form of configuration interaction (CI), a more accurate wave function is obtained by including the important intrashell mixing of $2s^2$ with $2p^2$,

$$\Psi^{CI} = c_1 1s2s^2(^2S) + c_2 1s2p^2(^2S). \tag{3}$$

The crucial aspect of this deviation from the single-configuration wave function is that the mixing coefficient c_2 is not small compared with unity. Using AUTOSTRUCTURE (Badnell 1986), our calculations reveal that the mixing coefficient c_2 varies from 0.34 for Be II to 0.32 for Zn XXVIII. It is of interest to note that the mixing is nearly constant over a broad range of ions along the isoelectronic sequence. The result of this significant mixing with the $1s2p^2$ configuration is that now there can be a substantial probability for this state to decay radiatively, that is, $\omega_K^{CI} \neq 0$.

Starting with this CI wave function Ψ^{CI}, AUTOSTRUCTURE was employed to calculate the various possible radiative and Auger rates and, subsequently, the fluorescence yields. The calculations were actually carried out using intermediate coupling to include spin-orbit effects, which become important as the nuclear charge Z increases. All three-electron systems from Be II to Zn XXVIII were considered.

3. RESULTS AND DISCUSSION

The results of our calculations for the K-shell fluorescence yield, ω_K, are tabulated in Table 1 and shown in Figure 1. It is clear that at the low-Z end, the fluorescence yield remains negligible, although not quite zero. With increasing Z, however, ω_K is no longer negligible, rising to a value of almost 0.18 for Zn XXVIII. In addition, a significant value of 0.118 is seen for the astrophysically important Fe XXIV ion. This is in good agreement with the multiconfiguration Breit-Pauli result of 0.116 given by Bautista et al. (2003) using the same code AUTOSTRUCTURE, and in fair agreement (≈10%) with the multiconfiguration Dirac-Fock result of 0.105 given by Chen (1986). This same ≈10% agreement is also found between our results and those given by Chen (1986) for C IV, N V, O VI, F VII, Ne VIII, Mg X, Si XII, Ar XVI, Ti XX, and Zn XXVIII.

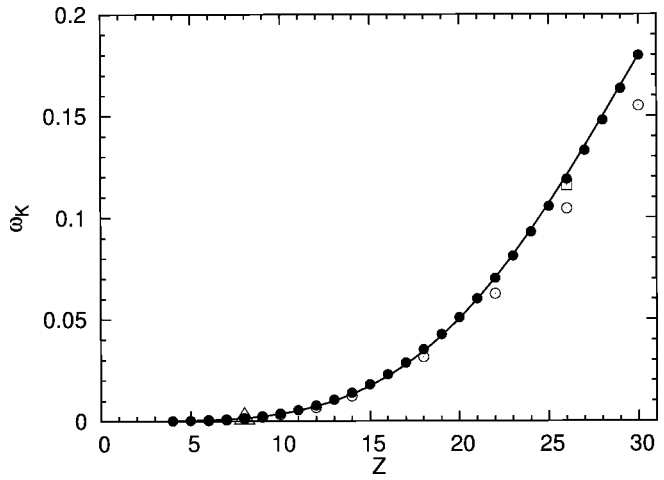

FIG. 1.—Calculated fluorescence yields ω_K^{CI} (*filled circles*) and fitted formula ω_K^{fit} from eq. (4) (*solid line*) for K-shell vacancy Li-like $1s2s^2$ ions. Also shown are the AUTOSTRUCTURE result for Fe XXIV (Bautista et al. 2003, *open square*) and the multiconfiguration Dirac-Fock (MCDF) results for C IV, N V, O VI, F VII, Ne VIII, Mg X, Si XII, Ar XVI, Ti XX, Fe XXIV, and Zn XXVIII (Chen 1986, *open circles*). On the scale of the figure, the MCDF results for C IV, N V, O VI, F VII, and Ne VIII overlap our results. The AUTOSTRUCTURE result for O VI (García et al. 2005, *open triangle*) was inferred from their $1s2p^2(^2S_{1/2})$ result by multiplying that value by c_2^2/c_1^2 (see text).

The more recent result of García et al. (2005) for the $1s2p^2(^2S_{1/2})$ state of O VI, $\omega_K = 0.0086$, can be used to infer the $1s2s^2(^2S_{1/2})$ value; according to equation (3), and considering that the $1s2p^2(^2S_{1/2})$ state is orthogonal to the $1s2s^2(^2S_{1/2})$ state, the ratio of the two fluorescence yields should be $\omega_K(1s2s^2)/\omega_K(1s2p^2) = c_2^2/c_1^2 = 0.1307$ for $c_2 = 0.34$. This gives a fluorescence yield for the $1s2s^2(^2S_{1/2})$ state of 0.0013, which is in good agreement with the present result of 0.0015. All the above results are in stark contrast to the currently used values of Kaastra & Mewe (1993), which are all zero.

The physics underlying the Z-dependence of ω_K, seen in Figure 1, can be explained in a relatively simple manner. To begin with, the Auger rate, A_A, is approximately independent of Z whereas the radiative rate, A_r, scales as $\sim Z^4$, within the framework of LS coupling (Cowan 1981). With increasing Z, however, the spin-orbit interaction becomes increasingly important and perturbs the Z^4 dependence of A_r with a small, negative contribution that scales as $\sim Z^7$. This suggests that the fluorescence yield $\omega_K \equiv A_r/(A_r + A_A) = 1/[1 + 1/(A_r/A_A)]$ can be well approximated by the fitting formula

$$\omega_K^{fit} \approx \left(1 + \frac{1}{aZ^4 - bZ^7}\right)^{-1}. \tag{4}$$

Fitting the above functional form to our calculated ω_K^{CI}, we obtain $a = 3.57 \times 10^{-7}$ and $b = 3.2 \times 10^{-12}$. The resulting ω_K^{fit} is shown in Figure 1 and tabulated in Table 1. The agreement with ω_K^{CI} is seen to be quite good except at very low Z, where the fluorescence yield is negligible anyway. This disagreement occurs because the approximate scaling is invalid at such low Z. It is to be emphasized that this fitting is based on the important physics for $Z \leq 30$; for higher Z, the above perturbative approach for the spin-orbit interaction is inaccurate and the fitting formula (eq. [4]) breaks down. In any event, since the $1s2p^2 \rightarrow 1s^22p$ radiative rate eventually dominates the Auger rate, the asymptotic $Z \rightarrow \infty$ fluorescence yield ω_K is equal to

TABLE 2

SUMMED OSCILLATOR STRENGTHS FOR THE $1s2p^2(^2S_{1/2}) \rightarrow \sum_{j=1/2}^{3/2} 1s^2 2p(^2P_j)$ RADIATIVE TRANSITIONS

Atomic Description	gf_L	gf_V
Without $1s2s2p(^4P)$ mixing	0.0141	0.0201
With $1s2s2p(^4P)$ mixing	0.0203	0.0201

NOTE.—Oscillator strengths gf are given in both length and velocity forms with and without the inclusion of the $1s2s2p(^4P)$ configuration mixed into the final state.

unity, in sharp contradistinction to the Kaastra & Mewe (1993) value of zero.

Another example of the large effect CI can have on the computed $1s2p^2 \rightarrow 1s^22p$ fluorescence yield is that the $1s^22p(^2P)$ final decay state mixes with the $1s2s(^3S)2p(^4P)$ configuration, by means of the spin-orbit interaction. In contrast, the $1s2s(^{1,3}S)2p(^2P)$ configurations do not mix appreciably with the $1s^22p(^2P)$ final decay state by the electrostatic interaction, as a consequence of Brillouin's theorem (Brillouin 1932; Cowan 1981). Now even though the mixing of the state $c_1 1s^22p_j(^2P) + c_2 1s2s(^3S)2p(^4P_j)$ is quite small ($c_2 \approx 0.008$), we find that the additional contribution from the $\langle 2p|\boldsymbol{D}|2s\rangle$ radial matrix element is much larger than the $\langle 2p|\boldsymbol{D}|1s\rangle$ radial matrix element when the dipole operator is expressed in the length form ($\boldsymbol{D} = \boldsymbol{r}$), although the reverse is true when it is instead expressed in the velocity form ($\boldsymbol{D} = \boldsymbol{\nabla}$). The contribution to the total dipole matrix element due to the inclusion of the $1s2s(^3S)2p(^4P_j)$ configuration is much greater in the length form than in the velocity form. As a matter of fact, the length form of the oscillator strength is not converged until this additional configuration is included in the atomic description, whereas the velocity form is converged even with this additional inclusion (see Table 2). The problem of which to use, length or velocity, is an old one (Chandrasekhar 1945; Starace 1982), and there is no really satisfactory solution except to perform a calculation that is accurate enough for the results to be equal in length and velocity forms.

In addition, it is evident that the dramatic modification of the fluorescence yields of three-electron, core-excited ions induced by many-body interactions is but an example of a much more general phenomenon. Configuration interaction can be of crucial importance in producing accurate atomic data in any situation where CI mixing leads to a transition that was completely forbidden in the absence of the mixing. Thus, while simple single-configuration calculations can sometimes be quite useful, for example, for inner shell photoionization cross sections well above threshold (Reilman & Manson 1979; Verner et al. 1993; Gorczyca et al. 2000), each situation must be judged individually to determine the possibility that many-body interactions might cause significant deviations from SC predictions.

Furthermore, these many-body interactions can result in CI that strongly modifies transitions that are not forbidden at the SC level. For example, in the dielectronic recombination (DR) of Na-like ions, there exists a significant $3s^2 + 3p^2$ intrashell correlation, which affects the rate coefficient in that it allows twice the number of accessible resonances, each with half the dielectronic capture rate and half the radiative rate, leading to a reduction by roughly a factor of 2 in the total DR rate coefficient. This was found in a theoretical study (Gorczyca & Badnell 1996) that explained why previous theoretical calculations were a factor of ≈2 larger than the experimental DR results for Fe XVI forming Fe XV (Linkemann et al. 1995). The work of Gorczyca & Badnell (1996) also explained the discrepancies between theory and experiment for the ion-atom process known as resonant transfer plus excitation (RTEX) of Nb XXXI (Bernstein et al. 1989) and Cu XIX and Cu XX (Závodszky et al. 1997).

4. SUMMARY

Many-body interactions in the form of configuration interaction are of crucial importance in the accurate calculation of a number of atomic properties relevant to astrophysics. The specific example of the K-shell fluorescence yields of core-excited Li-like ions was calculated; the inclusion of CI leads to significant values of the fluorescence yield as opposed to the single-configuration result of zero. For convenient astrophysical modeling, a two-parameter fit to the fluorescence yields is provided. It is expected that CI will be important in the accurate calculation of a variety of atomic processes occurring in astrophysical plasmas. Further work to delineate some of these situations is in progress.

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