Branching ratio of two-electron–one-photon transitions in doubly ionized low-Z atoms

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The branching ratio between the one-electron–one-photon and two-electron–one-photon transitions in doubly ionized K shells has been evaluated using an equivalent two-particle model with wave functions including angular correlations and relaxation in the length and velocity gauges. The accuracy of the results (choice of screening parameters and gauge dependence) will be discussed.

I. INTRODUCTION

In our previous Brief Report[1] we proposed a method for calculating the energies of the $K\alpha$-$K\alpha$ and $K\alpha_2^h$ lines using a two-particle model. These transitions are known to result mainly from relaxation. The role of angular correlation in two-hole states is an interesting aspect. Relaxation and angular correlation are both related to the correlated motion of electrons in many-electron systems. Our approach is based on two-electron wave functions that include the angular correlation explicitly but account for the relaxation by screening parameters. The determination of screening parameters is not based on *ab initio* principles. Instead, the screening has been tuned "by hand" so that the transition energies are in reasonable agreement with experimental values. This does not yet make the results useless or inconsistent, since it may be assumed that analogous to systems with two electrons outside a closed electron configuration, the angular correlation and relaxation (or screening) are to some extent independent of each other. However, the double-hole configurations in question interact strongly with other double-hole configurations of the same symmetry, which complicates the situation. The calculated (velocity gauge) branching ratios in Table II are in reasonable agreement with some of the calculations and experimental data. The angular correlation contributes at the level of 24–32 %.

II. THEORY OF BRANCHING RATIO BETWEEN $K\alpha_2^h$ AND $K\alpha$-$K\alpha$ TRANSITIONS

The transition rate of a dipole transition in the length gauge is given by

$$W_L = \tfrac{4}{3}\alpha^3(\Delta E)^3 |\langle \Psi_i | D | \Psi_f \rangle|^2 . \quad (1)$$

Here Ψ_i and Ψ_f denote the initial and final wave functions. α is the fine-structure constant, ΔE is the transition energy, and D is the dipole operator. The quantities appearing in Eq. (1) are in atomic units. In our two-particle model, the matrix elements of x and y components of the dipole operator are zero, as the angular part of the integral in each case vanishes after using Breit's[2] transformation formula. The transition rate of a dipole transition in the velocity form is given by

$$W_v = \tfrac{4}{3}\alpha^3(\Delta E) \left| \left\langle \Psi_i \left| \frac{\partial}{\partial Z_1} + \frac{\partial}{\partial Z_2} \right| \Psi_f \right\rangle \right|^2 .$$

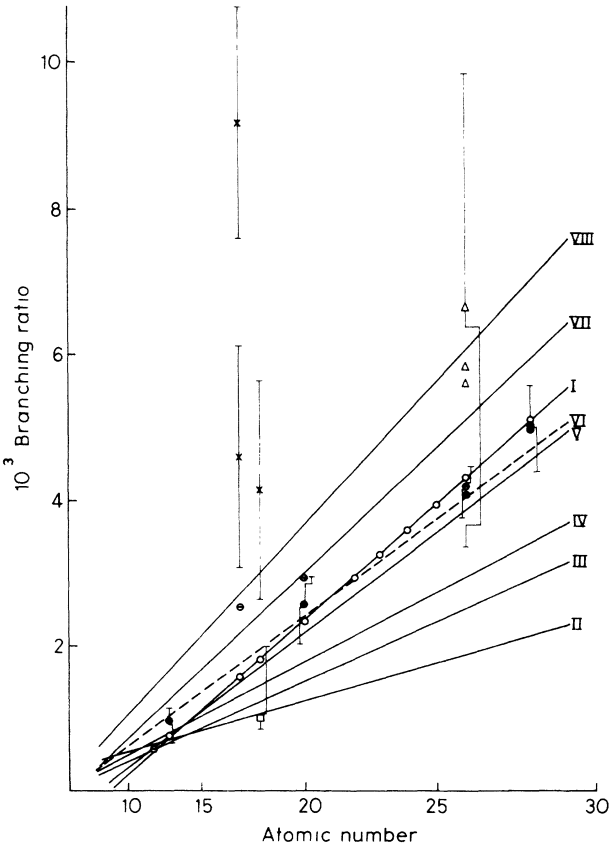

FIG. 1. Plot of branching ratio vs the square of atomic number. Theory: I, present work; II, Gavrila and Hansen (Ref. 10); III, Aberg, Jamison, and Richard (Ref. 5); IV and VIII, Safronova and Senashenko (Ref. 8); V, Baptista (Ref. 12); VI, Khristenko (Ref. 9); VII, Stoller (Ref. 7); ⊖, Kagawa (Ref. 11); △, Kelly (Ref. 6). Experiment: ⊗, Stoller *et al.* (Ref. 7); □, Knudson *et al.* (Ref. 13); △, Luken, Greenberg, and Vincent (Ref. 4); ×, Schuch, Gaukler, and Schmidt-Bocking (Ref. 14).

TABLE I. Values of the $K\alpha_2^h$ and $K\alpha$-$K\alpha$ rates (sec^{-1}). (i) indicates values with correlation, while (ii) indicates values without correlation. Figures in brackets indicate powers of 10.

Element		$K\alpha_2^h$ rate		$K\alpha$-$K\alpha$ rate		Energy (a.u.)	
		Length	Velocity	Length	Velocity	$K\alpha_2^h$	$K\alpha$-$K\alpha$
Mg	(i)	1.0353[13]	8.3950[12]	3.301[10]	1.343[10]	50.7506	97.8258
	(ii)	1.038[13]	8.347[12]	1.111[10]	1.086[10]	50.738 98	97.9398
Al	(i)	1.547[13]	1.275[13]	4.043[10]	1.628[10]	59.7972	115.676
	(ii)	1.551[13]	1.268[13]	1.281[10]	1.232[10]	59.7856	115.7935
Cl	(i)	5.588[13]	4.810[13]	7.833[10]	3.048[10]	103.4908	202.0837
	(ii)	5.597[13]	4.790[13]	2.521[10]	2.458[10]	103.4792	202.2132
Ar	(i)	7.279[13]	6.311[13]	9.021[10]	3.501[10]	116.291	227.3997
	(ii)	7.285[13]	6.286[13]	2.889[10]	2.823[10]	116.2794	227.5309
Ca	(i)	1.190[14]	1.050[14]	1.165[11]	4.499[10]	144.0601	282.5318
	(ii)	1.192[14]	1.046[14]	3.697[10]	3.627[10]	144.0485	282.6661
Ti	(i)	1.842[14]	1.647[14]	1.461[11]	5.622[10]	174.8293	343.6641
	(ii)	1.844[14]	1.641[14]	4.627[10]	4.526[10]	174.8179	343.8008
V	(i)	2.252[14]	2.026[14]	1.621[11]	6.224[10]	191.339	376.4803
	(ii)	2.255[14]	2.019[14]	5.100[10]	5.015[10]	191.3276	376.6179
Cr	(i)	2.727[14]	2.466[14]	1.789[11]	6.868[10]	208.5987	410.7965
	(ii)	2.731[14]	2.459[14]	5.617[10]	5.531[10]	208.5873	410.9351
Mn	(i)	3.274[14]	2.974[14]	1.967[11]	7.541[10]	226.6085	446.6128
	(ii)	3.278[14]	2.965[14]	6.161[10]	6.07[10]	226.5967	446.7521
Fe	(i)	3.899[14]	3.557[14]	2.153[11]	8.239[10]	245.3682	483.929
	(ii)	3.902[14]	3.546[14]	6.276[10]	6.635[10]	245.3568	484.0691
Ni	(i)	5.408[14]	4.970[14]	2.548[11]	9.737[10]	285.1378	563.0616
	(ii)	5.415[14]	4.958[14]	7.936[10]	7.837[10]	285.1264	563.203

The $1s^{-2}(^1S)$ state associated with the $K\alpha_2^h$ and $K\alpha$-$K\alpha$ lines is represented by the following function:

$$\Psi_0=\frac{\sqrt{2}}{4\pi}N_0F_0 ,$$

where $F_0=\exp[-a_0(r_1+r_2)/2](1+C_0\cos\theta)$,

$$N_0^2=\frac{1}{\int F_0^2 dv_{r_1,r_2;\theta}} ,$$

and $dv_{r_1,r_2;\theta}=r_1^2r_2^2\sin\theta\, dr_1 dr_2 d\theta$; θ is the angle between r_1 and r_2.

Following the procedure of Breit[2] the wave function for the $1s^{-1}2p^{-1}(^1P)$ state associated with the $K\alpha_2^h$ line can be written as

$$\Psi_1=\frac{\sqrt{6}}{4\pi}N_1(F_1\cos\theta_1+\tilde{F}_1\cos\theta_2) ,$$

where

$$N_1^2=\frac{1}{\int (F_1^2+2F_1\tilde{F}_1\cos\theta+\tilde{F}_1^2)dv_{r_1,r_2;\theta}} ,$$

$$F_1=r_1(1+C_1\cos\theta)\exp\left[\frac{-a_1r_1}{2}-\frac{b_1r_2}{2}\right] ,$$

$$F_1(r_1,r_2;\theta)=\tilde{F}_1(r_2,r_1;\theta) .$$

Similarly, the radial wave function for the $2s^{-1}2p^{-1}(^1P)$ state associated with the $K\alpha$-$K\alpha$ line is

$$F_2=r_1\left[1-\frac{b_2r_2}{2}\right](1+C_2\cos\theta)\exp\left[-\frac{a_2r_1}{2}-\frac{b_2r_2}{2}\right] .$$

Here, a_0,a_1,a_2,b_1,b_2 are the screening constants which have been computed using procedure of Burns[3] and C_0,C_1,C_2 are the variation parameters.

The appropriate transition rates are evaluated in the length and velocity gauges, both including and excluding angular correlations (Table I). The comparison of the theoretical and the experimental branching ratios is given in Table II. In Fig. 1 the calculated branching ratios in the velocity gauge, including angular correlation along with experimental values and different theoretical results, are presented as a function of the atomic number on a quadratic scale.

III. DISCUSSION

Table I shows that the effect of angular correlation is not appreciable when one calculates the energy of the $K\alpha$-$K\alpha$ line or $K\alpha_2^h$ line with two-particle wave function. However, the effect of angular correlation is appreciable in the case of the transition rate of the $K\alpha$-$K\alpha$ line with the two-particle model. In both gauges the $K\alpha_2^h$ transition rate is almost independent of angular correlation. For the $K\alpha$-$K\alpha$ line the angular correlation is significantly important, as expected, since the $K\alpha$-$K\alpha$ line originates out of a correlated jump of two electrons. From Table I, it is evident that in the length approximation, the $K\alpha$-$K\alpha$ rate decreases drastically when angular correlation is neglected. Consequently without angular correlation the branching ratio between the $K\alpha_2^h$ and the $K\alpha$-$K\alpha$ lines is larger than the values incorporating angular correlation in the length approximation (Table II).

The difference of $K\alpha_2^h$ rates in the two gauges decreases

TABLE II. Comparison of branching ratio. (i) indicates values with angular correlation, while (ii) indicates values without angular correlation.

Element	Present Velocity	Present Length	Previous Length	Previous Velocity	Previous Mixed	Experimental ratio
Mg	(i) 625	314	574[a]			
	(ii) 769	934	576[b]			
Al	(i) 783	383	1250,[c] 1020[d]			965±180[c]
	(ii) 1029	1211	682,[e] 667[a]			
Cl	(i) 1578	713	1109[a]			4600±1530[f]
	(ii) 1949	2220	1498[b]			9200±1600[f]
Ar	(i) 1803	807	1237,[a] 1950[d]			1000[h]
	(ii) 2227	2522	1668,[b] 1559[g]	5169[g]	2523[g]	4140±1500[f]
Ca	(i) 2334	1021	3000,[c] 1770[i]			2570±380[c]
	(ii) 2884	3224	2400,[d] 1240[e]			
			1515,[a] 2140[b]			
			1796[g]	6054[g]	2932[g]	
Ti	(i) 2930	1261	1820[a]			
	(ii) 3626	3985	2677[b]			
V	(i) 3255	1389	1984[a]			
	(ii) 4026	4422	2964[b]			
Cr	(i) 3591	1524	2155[a]			
	(ii) 4446	4862	3266[b]			
Mn	(i) 3944	1664	2332[a]			
	(ii) 4885	5321	3580[b]			
Fe	(i) 4317	1811	5100,[c] 2951[i]			4100±400[c]
	(ii) 5344	5801	4060,[d] 1870[e]			
			2518,[a] 3910[b]	8789[g]	4215[g]	
			2541[g]			
Ni	(i) 5104	2122	5800,[c] 3413[i]			5000±600[c]
	(ii) 6326	6823	4710,[d] 2120[e]			6680±3300[j]
			2909,[a] 4608[b]			
			2989[g]	10380[g]	4979[g]	

[a]Reference 5.
[b]Reference 12.
[c]Reference 7.
[d]Reference 9.
[e]Reference 10.
[f]Reference 14.
[g]Reference 11.
[h]Reference 13.
[i]Reference 8.
[j]Reference 4.

from Mg to Ni (within 7–23 % relative to the values in the velocity gauge). Without angular correlation the $K\alpha$-$K\alpha$ rate is almost independent of the choice of gauge (within 8–21 % relative to the values in the velocity gauge). However, the $K\alpha$-$K\alpha$ rate shows a large gauge dependence when we include angular correlation in the wave function (50–60 % of the values relative to the velocity gauge, Table II). According to Luken, Greenberg, and Vincent[4] the length and velocity results may be uncertain by as much as ±50% because of the importance of cancellations within the transition moment. Such cancellations occur only in the length formulation, and not in the velocity form. The neglect of angular correlation in a two-particle model yields values of branching ratio larger than the experimental values in both gauges (Table II).

The two-electron–one-photon transition rate is remarkably sensitive to the choice of screening parameters, because the $1s$ orbital in the $1s^2$ state is not orthogonal to the $2s$ orbital in the $2s2p$ state. Aberg, Jamison, and Richard[5] and Kelly[6] also arrived at the same conclusion. For Al, we have calculated the $K\alpha$ transition rate using the screening parameters for the $2s$ electron based on the configuration $(1s^0 2s^1 2p^6 3s^2 3p^2)$. For the $2p$ electron the configuration is $(1s^0 2s^2 2p^5 3s^2 3p^2)$. The two-electron–one-photon transition energy is not appreciably sensitive to the choice of the screening parameters.

Stoller *et al.*,[7] Safronova and Senashenko,[8] and Khristenko[9] calculated the transition rate of the $K\alpha$-$K\alpha$ and $K\alpha_2^h$ lines using two-electron wave functions in the length gauge only. According to Stoller *et al*[7]. the good agreement between the theoretical and experimental branching ratio is fortuitous. The agreement was possibly due to different inaccuracies in the approximation used that might cancel when the matrix element is calculated. The present branching-ratio values without angular correlation in length gauge agree fairly well with the calculated values of Stoller *et al.*[7] (Table II). Stoller *et al.*[7] neglected the effect of angular correlation between two electrons.

Safronova and Senachenko[8] used the first-order perturbation theory in the interelectron interaction for the initial and final wave functions. Neither of the authors took into account the effect of relaxation. The present

branching-ratio values including angular correlation in the length gauge are in reasonable agreement with the calculated values of Safronova and Senashenko.[8] (Table II). Safronova and Senashenko[8] considered a different transition $2s2p(^1P) \rightarrow 1s2s(^1S)$ in place of the present $K\alpha_2^h$ line. The method of Khristenko[9] is essentially equivalent to that used by Safronova and Senashenko.[8] Khristenko[9] obtained larger values for the branching ratio than those of Safronova and Senashenko[8] (Fig. 1, lines IV and VI). According to Stoller *et al.*[7] the $K\alpha$-$K\alpha$ satellite line could not be resolved and the charge state of ions resulting from collisions was not monitored. Therefore, a final comparison with experiment will have to wait until more is known about the initial population distribution in heavy-ion atom collisions. However, in view of the above-mentioned difficulties, it is not possible to rule out one of the calculations. Present branching-ratio values with angular correlation in the length gauge are also in reasonable agreement with those of Aberg *et al.*[5] (Table II). The formula used by Gavrila *et al.*[10] is same as that of Aberg, Jamison, and Richard.[5] Unlike Gavrila and Hansen,[10] Aberg, Jamison and Richard[5] set the integrals (overlap) equal to 1. Both authors used single-particle Hartree-Fock (HF) wave functions.

Kagawa[11] calculated the branching ratio of $K\alpha$-$K\alpha$ ($1s^{-2}$-$1s^{-1}2p_{1/2}^{-1}$) transitions using relativistic HF-Roothan wave functions in different gauges. His results in the velocity gauge were too high and in the length gauge too low. He devised a mixed gauge and obtained reasonably good values of the branching ratio. His results, however, deviated from the usual Z^2 dependence (Fig. 1). Baptista[12] considered the two-electron–one-photon decay process as a result of interaction between the jumping electrons and their interaction with the radiation field. The calculation was performed in second-order perturbation theory and the many-particle states were constructed from single-particle solutions. He obtained good agreement with experimental values. The branching ratio depends strongly on the initial configurations of the decaying atom. When calculating the energy of the $(2s2p)_{Z+1}$ state, the dependence on the initial configuration ($1s^{-2}$) of the decaying atom is considered through the screening parameter used to write the single-electron wave function. Kelly,[6] using the method of many-body perturbation theory, has obtained a branching ratio of 5630 (length) and 5860 (velocity) for Fe (Fig. 1).

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