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L-shell internal excitation accompanying L-capture

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Abstract. The L-shell internal excitation accompanying L-capture has been treated relativistically by the use of hydrogenic wave functions. Numerical calculations for the nuclides ^{37}Ar, ^{55}Fe, ^{77}Ge, ^{131}Cs, ^{157}Tb, ^{165}Er, ^{179}Ta and ^{193}Pt have been performed for the first-time. The present calculations show that double L_i-hole production probability decreases with increasing atomic number and it is almost independent of transition energy for a particular shell. Possible experiments to detect this phenomenon in atoms for which K-K processes are energetically forbidden are discussed briefly.

Keywords. Internal excitation; internal ionisation; K-capture; L-capture; double hole production.

1. Introduction

The process in which an atomic electron is excited during nuclear radioactive decay by capture of an orbital electron is known as a type of internal excitation. The first theoretical study of the process where the atom is excited during electron capture was made by Primakoff and Porter (1953). They used non-relativistic variational wave functions for the two electrons in the parent atom and obtained expressions for the double K-hole production probability. Recently internal excitation and ionisation accompanying K-capture has been investigated by Mukoyama *et al* (1973) using relativistic hydrogenic wave functions. Mukoyama and Shimizu (1974) calculated L_i-shell contributions to internal ionisation accompanying K- and L_i-electron capture. To date no theoretical work has been reported for L_i-shell contributions to internal excitation accompanying electron capture using relativistic hydrogenic wave functions.

In the present work, we report a more accurate relativistic treatment of the internal excitation of L_i-shell electrons accompanying L_i-capture, using an exact matrix element obtained from relativistic hydrogenic wave functions without any approximation. We have calculated both double K-hole and double L_i-hole production probabilities in typical nuclei and the double K-hole production probability of this work has been compared with earlier theoretical work and experimental measurements to test the consistency of present formalism.

2. General formulation

The transition probability of an orbital electron which is initially in the state ψ_i (Z, L_i), making a transition to a final state ψ_f (Z', n) during the capture of

another orbital electron $\psi'(Z, L_i)$ is expressed in terms of natural units ($\hbar = m = c = 1$) as

$$\omega = 2\pi \left| \langle \psi_f (Z', n) \psi_\gamma \psi_f(N) \left| H_\beta \right| \psi_i (N) \psi_i(Z, L_i) \psi' (Z, L_i) \rangle \right|^2 \rho (\nu, e), \quad (1)$$

where $\psi_i(N)$ and $\psi_f(N)$ are the initial and final nuclear wave functions, ψ_ν is the neutrino wave function, H_β is the weak interaction Hamiltonian and $\rho(\nu, e)$ is the density of final states. Separation of atomic and nuclear parts of equation (1) gives

$$\omega = 2\pi \left| \langle \psi_\nu \psi_f (N) \left| H_\beta \right| \psi_i (N) \psi' (Z, L_i) \rangle \right|^2 \times \left| \langle \psi_f (Z', n) \left| \psi_i (Z, L_i) \right\rangle \right|^2 \rho (\nu, e). \quad (2)$$

Here the first factor represents the nuclear matrix element part and the second factor represents atomic matrix element which is the overlap of the electron wave functions between initial and final states. The energy balance of electron capture decay is expressed, for equation (2) as

$$M_i + 2(1 - B_{L_i}) = M_f + q_\nu + (1 - B_n), \quad (3)$$

where M_i and M_f are the nuclear masses (in units of energy) in initial and final states, B_{L_i} and B_n are the binding energies of the electron in L_i and n state of the daughter atom and q_ν is the energy carried off by the neutrino. In calculating electron transition probabilities for L_i and higher shell electrons the atomic wave function overlap is usually neglected. As we are interested in L_i-shell internal excitation accompanying L_i-capture, the probability for L_i-electron capture is given by

$$\omega_{L_i} = \pi^{-1} G^2 g^2_{L_i}(R) \left| M_N \right|^2 S(W_0) W_0^2, \quad (4)$$

where the quantity G denotes the strength of the weak interaction, $g^2_{L_i}(R)$ is the density of L_i-electron at nuclear surface, M_N is the energy independent nuclear part of the matrix element, and $S(W_0)$ is the energy-dependent shape factor of the nuclear matrix element. The transition energy W_0 is

$$W_0 = M_i - M_f - B_{L_i} + 1. \quad (5)$$

Analogous to equation (4), the transition probability of the L_i-shell electron to the (ns) state of the daughter atom during L_i-capture is given by

$$\omega_{L_i n} = \pi^{-1} G^2 g^2_{L_i}(R) \left| M_N \right|^2 S(W_\nu) W_\nu^2 \left| M_{L_i n} \right|^2. \quad (6)$$

Here, $W_\nu = W_0 - B_{L_i} + B_n$ is the energy available to the neutrino, and

$$M_{L_i n} = \langle \psi_f (Z', n) \left| \psi_i (Z, L_i) \right\rangle$$

is the atomic wave function overlap of the L_i state of the parent with the (ns) state of the daughter. From equations (4) and (6), the probability per L_i-electron cap-

ture that the remaining L_i-electron in the parent atom undergoes a transition to the (ns) state of the daughter is

$$P_{L_in} = W_{L_in}/W_{L_i} = (W_\nu/W_0)^2 \ [S(W_\nu)/S(W_0)] \mid M_{L_in} \mid^2. \tag{7}$$

Let n'' be the highest occupied state of the parent atom; then the internal excitation probability per L_i-capture is

$$P_{\text{ex}} = \sum_{n=n''+1}^{\infty} P_{L_in}. \tag{8}$$

The completeness theorem states that

$$1 = \sum_{n=1}^{\infty} P_{L_in} + P_{ej}, \tag{9}$$

where P_{ej} represents total ionisation probability per L_i-capture. The probability for the double hole production in the L_i-shell of the daughter atom is

$$P(2) = P_{ex} + P_{ej} = 1 - \sum_{n=1}^{n''} P_{L_in} \tag{10}$$

In accordance with Primakoff and Porter (1953) $P(2)$ is expressed in terms of $P_{L_iL_i}$; the probability that the uncaptured L_i-electron still remains in the L_i-shell of the daughter, as

$$P(2) = \xi(1 - P_{L_iL_i}), \tag{11}$$

where ξ accounts for the occupied states of the daughter atom excluded by the Pauli principle.

3. Atomic matrix element for L_i-shell internal excitation

The atomic matrix element of the uncaptured L_i-shell electron in the parent atom making a transition to the (ns) state of the daughter atom is expressed as

$$M_{L_in} = \langle \psi_f (Z', n) \mid \psi_i (Z, L_i) \rangle, \tag{12}$$

where $\psi_i (Z, L_i)$ and $\psi_f (Z', n)$ represent respectively, the wave functions of the electron in the parent atom and daughter atom.

The L_i-shell coulomb wave functions of the parent atom can be written as

$$\psi_i (Z, L_i) = \begin{pmatrix} g_{-1} (\zeta_1, r) & \chi^{\mu}_{-1} (\hat{r}) \\ i f_{-1} (\zeta_1, r) & \chi^{\mu}_{1} (\hat{r}) \end{pmatrix} \quad \mu = \pm \tfrac{1}{2}, \tag{13}$$

where $\chi^{\mu}_1 (\hat{r})$ is the spin-angular function and the radial wave functions $g_{-1} (\zeta_1 r)$ and $f_{-1} (\zeta, r)$ are

$$g = N (1+W')^{1/2} r^{\gamma-1} \exp (-\lambda' r) (C_0 + C_1 r), \tag{14}$$

$$f = -N (1 - W')^{1/2} r^{\gamma-1} \exp (-\lambda' r) (a_0 + a_1 r). \tag{15}$$

Equations (14) and (15) represent the most general wave function for different shells, the respective factors like N, C_0, C_1, a_0, a_1, λ', W', etc. are explicitly given by Rose (1961).

The daughter atom wave function is given by (Rose 1961),

$$\psi_f(Z', n) = \begin{pmatrix} g_{-1}^{(n)}(r) & \chi_{-1}^{\mu}(\hat{r}) \\ i f_{-1}^{(n)}(r) & \chi_1^{\mu}(\hat{r}) \end{pmatrix}. \tag{16}$$

The radial wave functions $g_{-1}^{(n)}$ and $f_{-1}^{(n)}$ are

$$g_{-1}^{(n)}(r) = \frac{(2\lambda^5)^{1/2}}{\Gamma(2\gamma'+1)} \left[\frac{\Gamma(2\gamma'+n'+1)(1+W)}{n'!\,\zeta'(\zeta'-\lambda K)}\right]^{1/2}$$
$$\times (2\lambda r)^{\gamma'-1} \exp(-\lambda r)\,[-n' F(-n'+1, 2\gamma'+1, 2\lambda r)$$
$$-(K-\zeta'/\lambda) F(-n', 2\gamma'+1, 2\lambda r)], \tag{17a}$$

$$f_{-1}^{(n)}(r) = -\frac{(2\lambda^5)^{1/2}}{\Gamma(2\gamma'+1)} \left[\frac{\Gamma(2\gamma'+n'+1)(1-W)}{n'!\,\xi'(\xi'-\lambda K)}\right]^{1/2}$$
$$\times (2\lambda r)^{\gamma'-1} \exp(-\lambda r)\,[n' F(-n'+1, 2\gamma'+1, 2\lambda r)$$
$$-(K-\xi'/\lambda) F(-n', 2\gamma'+1, 2\lambda r)], \tag{17b}$$

where $\gamma'^2 = K^2 - \zeta'^2$, $\zeta' = aZ'$, $\lambda^2 = 1 - W^2$,

$W = (n'+\gamma')/[(n'+\gamma')^2 + \zeta'^2]^{1/2}$.

Here a- is the fine structure constant, $F(a, b, c)$ the confluent hypergeometric function, n' the radial quantum number, and K corresponds to the degenerate levels with same n and 1, given by

$$K = j_1 + \tfrac{1}{2} \quad \text{and} \quad K = -j_2 - \tfrac{1}{2}$$
$$(j_1 = l - \tfrac{1}{2},\ j_2 = l + \tfrac{1}{2}).$$

Using these initial and final electron wave functions, the overlap integral can be expressed as

$$\langle \psi_f(Z', n) | \psi_i(Z, L_i) \rangle = \int_0^{\infty} r^2\, dr\, [g_{-1}^{(n)}(r)\, g_{-1}(\zeta, r) + f_{-1}^{(n)}(r) f_{-1}(\zeta, r)]. \tag{18}$$

These radial integrals were solved by employing a method parallel to the one used by Jaeger *et al* (1935). Hence $M_{L_i n}$ becomes,

$$M_{L_i n} = \frac{2^{\gamma'-1/2}\,\lambda^{\gamma'+3/2}}{(\lambda+\lambda')^{\gamma+\gamma'+1}} \frac{\Gamma(\gamma+\gamma'+1)}{\Gamma(2\gamma'+1)} N \left[\frac{\Gamma(2\gamma'+n'+1)}{n'!\,\zeta'(\zeta'-\lambda K)}\right]^{1/2}$$
$$\times \Big\{ n'(-A_1 C_0 + A_2 a_0) F_1 - (K-\zeta'/\lambda)(A_1 C_0 + A_2 a_0) F_2$$
$$+ \frac{(\gamma+\gamma'+1)}{(\lambda+\lambda')} [n'(-A_1 C_1 + A_2 a_1) F_3 - (K-\zeta'/\lambda)(A_1 C_1 + A_2 a_1) F_4] \Big\}, \tag{19}$$

where $A_1 = [(1+W)^{1/2}\,(1+W')^{1/2}]$,

$A_2 = [(1-W)^{1/2}\,(1-W')^{1/2}]$.

and $F_1 = F(\gamma+\gamma'+1,\ -n'+1,\ 2\gamma'+1,\ 2\lambda/(\lambda+\lambda'))$,

$F_2 = F(\gamma+\gamma'+1,\ -n',\ 2\gamma'+1,\ 2\lambda/(\lambda+\lambda'))$,

$F_3 = F(\gamma+\gamma'+2,\ -n'+1,\ 2\gamma'+1,\ 2\lambda/(\lambda+\lambda'))$,

$F_4 = F(\gamma+\gamma'+2,\ -n',\ 2\gamma'+1,\ 2\lambda/(\lambda+\lambda'))$.

A typical matrix element for the L_i-electron remaining in the L_i-shell of the daughter atom may be written with the help of equation (19) as

$$M_{L_i L_i} = \frac{2^{\gamma+\gamma'-3/2}\,\lambda^{\gamma'+3/2}\,\zeta^{\gamma+1/2}}{C_0^{\gamma+1}\,(\lambda+\lambda')^{\gamma+\gamma'+1}}\,\frac{\Gamma(\gamma+\gamma'+1)}{\Gamma(2\gamma'+1)}$$
$$\times\left[\frac{\Gamma(2\gamma'+2)\,(2\gamma+1)}{\Gamma(2\gamma+1)\,(C_0+1)\,\zeta'(\zeta'+\lambda)}\right]^{1/2}\Big\{(P-Q)+(1+\zeta'/\lambda)$$
$$\times(P+Q)\,F(\gamma+\gamma'+1,\ -1,\ 2\gamma'+1,\ 2\lambda/(\lambda+\lambda'))$$
$$-\left(\frac{\gamma+\gamma'+1}{\lambda+\lambda'}\right)(2\zeta/C_0)\left(\frac{2C_0+1}{2\gamma+1}\right)[(R-S)+(1+\zeta'/\lambda)$$
$$\times(R+S)\,F(\gamma+\gamma'+2,\ -1,\ 2\gamma'+1,\ 2\lambda/(\lambda+\lambda'))]\Big\} \qquad (20)$$

where $P = (1-W)^{1/2}\,(2-C_0)^{1/2}\,(C_0+2)$, $Q = (1+W)^{1/2}\,(2+C_0)^{1/2}\,C_0$,

$R = P/C_0 + 2$, $S = R/C_0$.

Similar expressions may be obtained for L_2 and L_3-shell electrons.

4. Numerical results and discussion

In order to account for the effects of coulomb interaction and spatial correlation of the electrons, the nuclear charge Z in the hydrogenic wave functions was replaced by an appropriate effective nuclear charge $Z_{\text{eff}} = Z - \sigma$, where σ is known as the screening number. Froese (1972) has tabulated the values of σ for different nuclei and these were used to obtain the Z dependence of σ for the nuclides of interest. Considering *a* hole in the daughter atom due to electron capture, the screening number was calculated using the relation $\sigma_c = (\sigma_h/\sigma_s)\,\sigma$, where σ_h is the Slater's (1930) screening constant with a hole in L_i-shell, σ_s is that of the ordinary atom and σ is the screening number as calculated above. The difference of effective nuclear charge between parent and daughter atom (without a hole in L_i-shell) calculated by Mukoyama and Shimizu (1974) is almost constant, ranging from 0·97 to 0·98 for all L-subshells for nuclides ^{55}Fe, ^{71}Ge, ^{131}Cs and ^{165}Er. It is interesting to note that the difference of effective nuclear charge calculated in this work for nuclides ^{37}Ar, ^{55}Fe, ^{71}Ge, ^{131}Cs, ^{157}Tb, ^{165}Er, ^{179}Ta and ^{193}Pt is also almost constant ranging from 0·988 to 0·989 for all L-subshells.

We have calculated double hole production probabilities per K- and L_i electron capture for nuclides ^{37}Ar, ^{55}Fe, ^{71}Ge, ^{131}Cs, and ^{165}Er as double K hole production probabilities for these nuclides are known experimentally. In the case of ^{157}Tb, ^{179}Ta and ^{193}Pt nuclides only double L_i-hole production probabilities have been obtained, because double K-hole production probabilities for these nuclides have not been measured previously. For all these calculations the factor ξ in equation (11) was taken to be 2/3 and L_3 capture was considered to be negligible. All these calculations were performed with the aid of a computer. The nuclear parameters used for these nuclides were taken from Leaderer *et al* (1967). The probabilities $P(2)$ found in the present numerical calculations are summarised in table 1. For comparison both theoretical and experimental probabilities per K-capture of the double K-hole production are also given for five nuclides (^{37}Ar, ^{55}Fe, ^{71}Ge, ^{131}Cs and ^{165}Er).

The presently calculated double K-hole production probabilities for the above mentioned five nuclei compares reasonably with the theoretically calculated values of Mukoyama *et al* (1973) and experimental measurements (given in table 1 with references). This fact suggests that our results are consistent with the earlier work.

Table 1. Double hole production probabiilites per K and L_i capture.

Nuclide	Transition energy keV	Shell	Theoretical, 10^5 p(2) Present Work	TM(a)	Experimental 10^5 p(2)
^{37}Ar	814	K	31·69	23·0	44±8 (b) 37±9 (c)
		$L1$	364·44		
		$L2$	180·52		
^{55}Fe	231	K	14·51	15·8	14±2 (d)
		$L1$	144·44		
		$L2$	69·37		
^{71}Ge	235	K	11·03	8·85	13·3±1·4 (e) 13±8 (f)
		$L1$	89·53		
		$L2$	42·35		
^{131}Cs	381	K	4·24	1·79	5·10±1·0 (g) 2·5±0·2 (b)
		$L1$	27·68		
		$L2$	15·34		
^{165}Er	370	K	1·39	1·09	1·5±0·4 (h) 0·67±0·39 (i)
		$L1$	18·40		
		$L2$	7·90		
^{157}Tb	60	$L1$	19·87		
		$L2$	8·00		
^{179}Ta	100	$L1$	16·40		
		$L2$	7·47		
^{193}Pt	40	$L1$	14·87		
		$L2$	7·31		

(a) Tm refers to T Mukoyama *et al* (1973).
(b) Lark and Perlman (1960). (c) Kiser and Johnston (1959). (d) Briand *et al* (1974).
(e) Langevin *et al* (1957). (f) Oertzen (1964).
(g) Daniel *et al* (1960). (h) Ryde *et al* (1963). (i) Nagy *et al* (1972).

In some cases like ^{37}Ar and ^{131}Gs, our $P(2)$ values for K-shell differ as much as 30% from that of Mukoyama *et al* (1973). This is mainly due to the procedural variation in obtaining σ by Mukoyama *et al* (1973) and the present work.

The results show that L_i-internal excitation accompanying L_i-capture could be observed if the double L_i-hole production probability is large because the L_i-L_i process is almost of the same order of magnitude as the K-K process which has already been studied experimentally.

The double L_i-hole production probability accompanying L_i-electron capture decreases with increasing atomic number. Unlike internal ionisation probability accompanying electron capture which shows dependence on nuclear transition energy, the double L_i-hole production probability is found to be almost independent of nuclear transition energy for a particular shell, because this process is mainly an atomic phenomenon which does not affect nuclear energy.

In conclusion, the present results indicate that an experimental study on the L_i-L_i process should be possible because the double hole production probability for the L_i-L_i process is much greater than that of K-K process. The motivation for doing experimental work in this field is not necessarily to check the calculated values, but such experiments would aid the understanding of internal excitation of the atoms. Especially the nuclides ^{157}Tb, ^{179}Ta and ^{193}Pt are most suitable for this purpose because the K-K processes are energetically forbidden. The experimental method used for the study of the K-K process is still applicable to these nuclides namely L-x-ray-L-x-ray coincidence experiments.

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