Probability for K- and L-vacancy creation in electron-capture decay

M. C. Chon and J. Law
Guelph-Waterloo Program for Graduate Work in Physics, Guelph Campus, University of Guelph, Guelph, Ontario, Canada N1G 2W1
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The self-consistent-field model for K shakeoff in $\beta^{\pm}$ decay and electron-capture (EC) decay is extended to deal with the processes of L shakeoff accompanying K capture and K shakeoff accompanying L capture. The results indicate that many-body effects play an important role and reduce the shakeoff probability.

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I. INTRODUCTION

When the nucleus decays due to the weak interaction ($\beta^{\pm}$ and electron capture), the atomic electron cloud is disturbed. This may cause electronic excitation to unoccupied bound states (shakeup, SU) or ionization to the continuum states (shakeoff, SO), and the atomic system ends up with inner-shell vacancies. Most of the theoretical and experimental effort has been concentrated on the K-electron shakeoff probability. The measurable quantities which can be compared with the theory are the K-vacancy creation probability P_K in $\beta^{\pm}$ decay, and the two K vacancies creation probability P_{KK} in electron-capture (EC) decay.

In recent theoretical approaches, the discrepancy between the experimental data and the theoretical predictions in the K shakeoff accompanying $\beta^{\pm}$ decays have been essentially resolved. The self-consistent-field (SCF) one-step theory by Law and Suzuki [1] succeeded in explaining the group of experimental values quantitatively in the case of β^- decay, indicating that the atomic configuration in the final state should be properly chosen. On the other hand, Intemann [2] obtained a satisfactory agreement with measured P_K values in the case of β^+ decay taking into account the contribution from the direct collision (DC) between the emerging β particle and an atomic electron.

However, there remains a problem to be solved in the theory in EC decay in which some systematic deviations between experimental and theoretical P_{KK} exist. The two most sophisticated theoretical approaches, SCF theory by Suzuki and Law [3] and the semirelativistic-propagator (SRP) method by Intemann [4], bracket most of the measured values. (The experimental and theoretical situations are summarized in Ref. [5].) Obviously, further theoretical investigation on the electron-capture shakeoff is required.

The present paper is concerned with the processes, L shakeoff in K capture (L-SO in K-EC) and K shakeoff in L capture (K-SO in L-EC). Since both processes end up with K and L vacancies of a daughter atom, these processes can contribute to the electron-K-X-ray coincidence spectrum, which is used to measure the K-SO probability in K-EC. These processes have to be studied in order to remove the contributions from the L-shell electrons to the coincidence spectrum to obtain experimental P_{KK} values. The study of these processes can provide important information on shakeoff in EC decay.

Primakoff and Porter [6] suggested that K capture would give rise to no L shakeoff, since the L electrons are under the influence of approximately the same effective charge in the initial and the final states, because of the shielding by the K electrons. Wolfsberg [7], however, noted the significance of L-electron contributions to the coincidence spectrum. Following Wolfsberg's suggestion, several theoretical calculations have been done. Law and Campbell [8] calculated nonrelativistically the probability of L_1-SO in K-EC and K-SO in $L_1(2S_{1/2})$EC. Mukoyama and Shimizu [9] estimated the contributions from all L subshells, L_1, $L_2(2P_{1/2})$, and $L_3(2P_{3/2})$, using screened relativistic hydrogenic wave functions. They found that L-shakeoff probability is strongly influenced by the initial state correlation. In other words, the probability is very sensitive to the phenomenological screening parameter chosen.

In order to remove the ambiguity with respect to the phenomenological parameters, the SCF model is extended to calculate these processes.

II. FORMALISM

The formalism for K-SO in L-EC and L-SO in K-EC can be done in an analogous way to K-SO in K-EC [3]. For both processes, the initial state is a neutral atom in its ground state, and the final state is the 1^+ ion with one K and one L vacancy. Suppressing the nuclear and neutrino variables, we may take the initial and final states to be

$$|i\rangle = |\, e_{K_1}, e_{K_2}, e_{L_i} \,\rangle,$$

$$|f\rangle = |\, e'_p, e'_K \,\rangle.$$

The decay rate of the process is calculated following Fock space methods by Law and Campbell [10], and we have

$$\lambda_{KL_i-L_iK} = \frac{G_v^2}{\pi}\,\xi\,|\phi_K(0)|^2 \int \frac{d^3p}{(2\pi)^3}\,(W_{KL_i}-W_p)^2 \times\Big[\,|\langle e'_p|e_{L_i}\rangle|^2 + \frac{|\,\phi_{L_i}(0)\,|^2}{|\,\phi_K(0)\,|^2}|\langle e'_p|e_K\rangle|^2 -\delta_{i,1}\,\mathrm{Re}\left(\frac{\phi_{L_i}(0)}{\phi_K(0)}\,\langle e'_p|e_K\rangle\langle e_{L_i}|e'_p\rangle\right)\Big], \tag{2.1}$$

where G_v is the vector coupling constant, ξ is the allowed combination of nuclear matrix element, W_{KL_i} is the transition energy in this process, and W_p is the total energy of the continuum electron. (We use units in which $\hbar = c = 1$.) The coefficient in front of the interference term (the last term in the square brackets) is 1 instead of 2 after spin averaging of the initial K- and L-shell electrons. We can define the shakeoff probability of L-SO in K-EC and K-SO in L-EC per K capture as

$$P_{KL_i-L_iK} = \frac{\lambda_{KL_i-L_iK}}{\lambda_{\mathrm{EC}}}, \tag{2.2}$$

where λ_{EC} is the K-capture rate,

$$\lambda_{\mathrm{EC}} = \frac{G_v^2}{\pi}\,\xi\,|\,\phi_K(0)\,|^2\,W_0^2. \tag{2.3}$$

It is important to note that two processes, L_1-SO in K-EC and K-SO in L_1-EC, cannot be distinguished. For both cases, the final continuum states have the single particle angular quantum number $\kappa = -1(S_{1/2})$. Therefore, we have an interference term in $P_{KL_1-L_1K}$. On the other hand, there is no interference term for L_i $(i = 2,3)$. In principle, it is possible to distinguish them. However, the angular distribution of the electron has not yet been measured experimentally, so all the processes have to be considered together. The total contribution from the L shell is given by

$$P_L = \sum_{i=1}^{3} P_{KL_i-L_iK}. \tag{2.4}$$

For discussion purposes, we define the L_i-shakeoff probability as

$$P_{KL_i} = \frac{\lambda_{KL_i}}{\lambda_{\mathrm{EC}}}, \tag{2.5}$$

$$\lambda_{KL_i} = \frac{G_v^2}{\pi}\,\xi\,|\phi_K(0)|^2 \times\int \frac{d^3p}{(2\pi)^3}\,(W_{KL_i}-W_p+m_e)^2\,|\langle e'_p|e_{L_i}\rangle|^2. \tag{2.6}$$

We also define the K-shakeoff probability during L_i-capture per ordinary K capture as

$$P_{L_iK} = \frac{\lambda_{L_iK}}{\lambda_{\mathrm{EC}}}, \tag{2.7}$$

$$\lambda_{L_iK} = \frac{G_v^2}{\pi}\,\xi\,|\phi_K(0)|^2 \int \frac{d^3p}{(2\pi)^3}\,(W_{KL_i}-W_p+m_e)^2 \times\frac{|\phi_{L_i}(0)|^2}{|\phi_K(0)|^2}|\langle e'_p|e_K\rangle|^2. \tag{2.8}$$

The study of K-SO during β^- decay indicates that the whole system undergoes rearrangement to a fully relaxed state. Therefore the transition energy of the processes can be obtained by comparing the initial and final energies of the whole system including all the remaining electrons. For the initial state,

$$E_i = M_a(Z+1,A), \tag{2.9}$$

where M_a is the atomic mass whose nuclear charge is $Z+1$ and mass number is A. For the final state,

$$E_f = M_n(Z,A) - B_{KL_i}(Z) + (Z-1)m_e + W_p + q_\nu, \tag{2.10}$$

where B_{KL_i} is the total binding energy of the 1^+ ion with both K and L vacancies. Therefore the transition energy can be written as

$$W_{KL_i} = W_p + q_\nu = Q_{\mathrm{EC}} - [B(Z) - B_{KL_i}(Z)], \tag{2.11}$$

where Q_{EC} is the tabulated Q value of the decay and $B(Z)$ is the total binding energy of the neutral atom.

The main difficulty in calculating the decay rates lies in the evaluation of the overlap integrals. In most of the theoretical calculations, hydrogenic wave functions (relativistic or nonrelativistic) with screening parameters are used to evaluate the overlap integrals. In the SCF theory, the initial state wave function is obtained from the Dirac-Fock-Slater (DFS) atomic structure program of Lindgren and Rosén [11]. The final continuum state is obtained by solving the DFS equation numerically with a SCF one-body potential. As seen in [1,3], the choice of atomic configuration is crucial. In the physical situation for L-SO in K-EC and K-SO in L-EC, the parent atom undergoes EC decay to a final state which consists of a 1^+ ion with both K and L vacancies, one neutrino, and one continuum electron. For example, in the case of the decay $^{55}_{26}\mathrm{Fe} \rightarrow {}^{55}_{25}\mathrm{Mn}$, we have

$$\mathrm{Fe} \rightarrow \mathrm{Mn}^+ + e^- + \nu_e,$$

$$\{[\mathrm{Ar}]4s^2\ 3d^6\}_{26} \rightarrow \{[\mathrm{Ar}](K^{-1}L^{-1})\ 4s^2\ 3d^6\}_{25} + e'_p + \nu_e,$$

where the explicit configuration has been written down in the second form. The subscripts of the terms in curly brackets stand for the nuclear charge. The SCF potential for the continuum wave function is obtained from the DFS program with this configuration.

III. NUMERICAL RESULTS AND DISCUSSION

The shakeoff probability $P_{KL_i-L_iK}$ was calculated for nuclides ^{37}Ar, ^{55}Fe, ^{71}Ge, ^{131}Cs, and ^{165}Er using Eq. (2.2). In addition, L_i-SO probability in K-EC, P_{KL_i}, and

TABLE I. Shakeoff probabilities (in units of 10^{-5}) in K-capture decay for ^{55}Fe calculated with the SCF wave functions from (a) one K and one L vacancy, (b) one K vacancy, and (c) one L vacancy. For comparison, the results with Dirac wave functions (Dirac) and those obtained by Mukoyama and Shimizu (MS) are also listed.

Quantity	Dirac	SCF (a)	SCF (b)	SCF (c)	MS
P_{KL_1}	78.5	35.1	59.26		11
P_{L_1K}	4.99	4.06		8.03	11
P_{KL_2}	32.58	1.657	15.34		0.084
P_{L_2K}	0.027	0.023		0.445	
P_{KL_3}	30.89	1.607	14.38		0.069

K-SO probability in L_i-EC per K capture, P_{L_iK}, were calculated using Eq. (2.5) and Eq. (2.7), respectively. Nuclear and atomic data were taken from Ref. [12].

The results obtained for ^{55}Fe are displayed in Table I under the heading SCF. To see the effect of the inner-shell vacancies, these values were calculated for three different configurations:

$$\text{(a)}\ [\text{Ar}](K^{-1}L_i^{-1})4s^2 3d^6,$$

$$\text{(b)}\ [\text{Ar}](K^{-1})4s^2 3d^6,$$

$$\text{(c)}\ [\text{Ar}](L_i^{-1})4s^2 3^6.$$

For comparison, we also have listed the theoretical results obtained by Mukoyama and Shimizu [9] under the heading MS. Also of interest are the results obtained by employing hydrogenic Dirac wave functions (labeled Dirac) for both electronic states, completely neglecting all correlation and screening effects. As was observed in the case of K-SO in K-EC, P_{KK} obtained by using Dirac wave functions is larger than the SCF values. The dramatic reduction in P_{KL_i} which results when the Dirac wave function is replaced by the SCF wave function is striking. This reduction is due to the smaller overlap between the initial bound state and the final continuum state in the SCF scheme. The use of the SCF potential, which takes into account all the remaining electrons, causes the continuum wave function to be pushed out and gives a smaller overlap with the initial bound state. This tendency is observed in all nuclides.

As far as P_{L_iK} is concerned, the discrepancy between the SCF values and MS values is attributed to the different final state configurations. In the MS work, the configuration (b) is used for P_{KL_i}, and (a) for P_{L_iK}. If the configuration with one L_i vacancy is used in the SCF model, the theoretical values are doubled and approach MS results. On the other hand, in the case of P_{KL_i}, SCF and MS values are so different that we cannot attribute the discrepancy only to the final state configuration. L-SO probabilities seem to be much more sensitive to the final state potential to be used. The problem is complicated by the effects coming from the many-body nature of the problem, so that it may not be reducible to a simple parametrization.

TABLE II. Shakeoff probabilities in units of 10^{-5}. See text for definitions of shakeoff probabilities.

Nuclide	P_{KL_1}	P_{L_1K}	$P_{KL_1-L_1K}$	P_{KL_2}	P_{L_2K}	P_{KL_3}	P_L
$^{37}_{18}$Ar	76.40	8.56	62.20	3.955	0.020	4.002	70.18
$^{55}_{26}$Fe	35.11	4.06	28.32	1.657	0.023	1.607	31.61
$^{71}_{32}$Ge	27.08	2.23	17.72	1.070	0.024	1.060	19.87
$^{131}_{55}$Cs	8.31	0.86	5.52	0.334	0.031	0.289	6.17
$^{165}_{68}$Er	5.27	0.67	4.131	0.248	0.036	0.150	4.57

The numerical results for all five nuclides are listed in Table II. P_{L_3K} has not been listed in the table, because L_3- to K-capture ratio is too small ($\sim 10^{-8}$) to contribute to $P_{KL_3-L_3K}$. In fact, for allowed decays, L_3 capture is forbidden. Due to the small overlap with the continuum state, the contributions from L_2 and L_3 shells are small ($\sim 10\%$) compared to the contribution from the L_1 shell, hence the dominant part of the L-shell contribution to the ionization process comes from the L_1 subshell.

It has been noted in the past that the shakeoff probability generally decreases with Z^{-2}. Omitting the Q-value dependence, we find from our calculation

$$P_{KL_1-L_1K} \simeq \left(\frac{136.4}{Z}\right)^2 \times 10^{-5}, \tag{3.1}$$

$$P_{KL_2-L_2K} \simeq \left(\frac{34.9}{Z}\right)^2 \times 10^{-5}, \tag{3.2}$$

$$P_{KL_3-L_3K} \simeq \left(\frac{34.3}{Z}\right)^2 \times 10^{-5}. \tag{3.3}$$

$$P_L \simeq \left(\frac{149.3}{Z}\right)^2 \times 10^{-5}. \tag{3.4}$$

Till now, our discussion has been restricted to the shakeoff probabilities. It is also of interest to observe the spectral distribution of the ejected electron. In Fig. 1, we have plotted the theoretical spectrum shape of the ejected electron for $^{55}_{26}$Fe. It can be seen that the L-shell contribution is significant over the whole energy range. In particular, in the low energy region, the contribution from the L-shell dominates the spectrum.

Experimental data are available only for P_L in ^{37}Ar. The experiment was performed by Neumann [13], who measured an electron spectrum composed of K-SO in K-EC, L-SO in K-EC, and K-SO in L-EC. In the energy range 4.1–5.0 keV, the experimental data were fitted using Levinger's theoretical spectrum shape for L-SO in K-EC [14] assuming that the spectrum contains important contributions only from L-SO in K-EC and K-SO in L-EC. The experimental value $P_L = 130 \times 10^{-5}$ was obtained by extrapolation. The value is inconsistent with our result, $P_L = 70.18 \times 10^{-5}$, and the result of Mukoyama and Shimizu, $P_L = 57 \times 10^{-5}$. However, it should be noted that Levinger's spectrum was obtained by employing a nonrelativistic hydrogenic wave function, which gives a larger shakeoff probability than the SCF result by up to a factor of 2. Moreover, since the L-shell contribution is significant in the whole energy region, one cannot separate out the L-shell contribution from K-shell ionization in K capture by measuring the double coincidence spectrum. Therefore we consider that it is premature to make a quantitative comparison between the experimental data and the theoretical calculations.

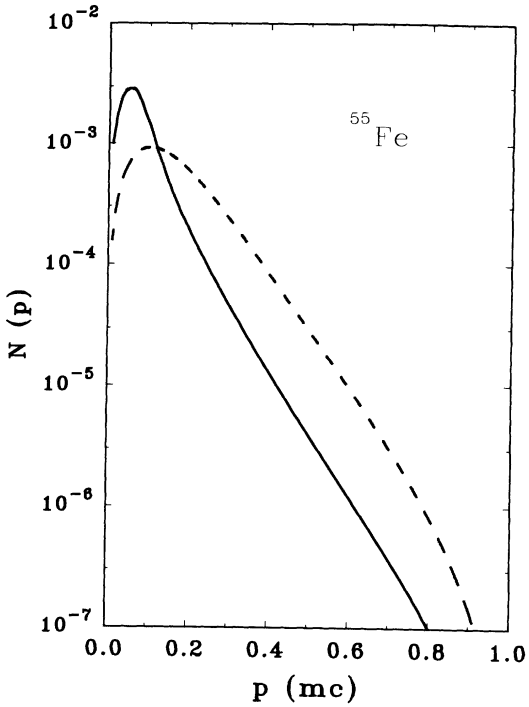

FIG. 1. Momentum spectrum of ejected electrons in ^{55}Fe. Solid line: the spectrum of ejected electrons for K-capture–L-shakeoff and L-capture–K-shakeoff; dashed line: K-capture–K-shakeoff.

Further experimental studies need to be made of the L-shell contributions to the inner-shell ionization accompanying electron capture. We hope that measurements of P_L will be forthcoming as they will provide an opportunity to make a quantitative comparison between the experimental values and the numerical results obtained in this work.

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