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Electron Shake-up and Shake-off Following ^{6}He Beta Decay

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Abstract. Probabilities for electron shake-up and shake-off are calculated as relaxation processes following the beta decay of ^{6}He to form ^{6}Li, including corrections due to nuclear recoil. Within the sudden approximation, it is found that the correction due to nuclear recoil is nearly an order of magnitude less than that measured by Carlson *et al.* Phys. Rev. **129**, 2220 (1963).

1 Introduction

There are currently several experiments in progress to search for new physics beyond the Standard Model by high precision studies of angular correlations in the $E_{\rm max} = 3.508$ MeV β decay of the helium isotope $^6\mathrm{He} \rightarrow {}^6\mathrm{Li} + e^- + \bar{\nu}_e$ [1, 2]. An essential part of the analysis is to understand the energy distribution and spectra of the recoil ions. After the β decay event, the atomic electrons suddenly find themselves in a $^6\mathrm{Li}^+$ environment with nuclear charge $Z = 3$. The electrons redistribute themselves over all possible states of the $^6\mathrm{Li}^+$ ion, including the continuum leading to $^6\mathrm{Li}^{++}$ and $^6\mathrm{Li}^{3+}$. Evidence for new physics beyond the Standard Model would reveal itself by an additional tensor coupling contribution to the weak interaction, in addition to the simple Gamow-Teller axial-vector mechanism [1–3]. We present here a brief summary of a more extensive discussion to be published elsewhere [4].

2 Theory and Calculations

The maximum β-particle momentum is $P_{\rm max} = 1070$ a.u., which is relativistic. However, because of its larger mass, the maximum recoil velocity of the $^6\mathrm{Li}^+$ nucleus is only $v_{\rm rec} = 0.09749$ a.u., which is nonrelativistic. If the initial state of the atom is taken to be at rest in the laboratory frame, then the atomic electrons with position vectors $\mathbf{r}_i$ relative to the nucleus have a maximum recoil momentum $K \equiv m_e v_{\rm rec} = 0.09749$ a.u. after β-decay. Since the operator $\exp(i\mathbf{K}\cdot\mathbf{r})$ generates the transformation to a moving frame of reference, Born's rule for the transition probability from an initial atomic state i of ^{6}He to a final atomic state f of $^6\mathrm{Li}^+$ with recoil momentum $\mathbf{K}$ is

$$P_{i\rightarrow f}(\mathbf{K}) = \left|\left\langle \Psi_i(^6\mathrm{He}) \left| e^{i\mathbf{K}\cdot\mathbf{r}} \right| \Psi_f(^6\mathrm{Li}) \right\rangle\right|^2 \tag{1}$$

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where $\mathbf{r} = \mathbf{r}_1 + \mathbf{r}_2$. Then by closure,

$$\sum_f P_{i\to f}(\mathbf{K}) = 1 \tag{2}$$

independent of $\mathbf{K}$, where the sum over f includes all bound and continuum states of Li^{++} and Li^{3+}, as well as Li^{+}. This sum rule will provide an important check on the final results.

Since $K = |\mathbf{K}|$ is small, it is convenient to use the multipole expansion (with z-axis in $\hat{\mathbf{K}}$ direction)

$$\begin{aligned} e^{i\mathbf{K}\cdot\mathbf{r}} &= e^{iKz} \\ &= 1 - \frac{(Kr)^2}{6} + iKz - \frac{(Kr)^2}{3}P_2(\cos\theta) + \cdots \end{aligned} \tag{3}$$

where $P_2(\cos\theta)$ is a Legendre polynomial inducing quadrupole transitions, and by definition $r^2 = |\mathbf{r}_1+\mathbf{r}_2|^2 = r_1^2+r_2^2+2\mathbf{r_1}\cdot\mathbf{r}_2$. The quadrupole term can be neglected because it is of order K^4 after squaring, but both the monopole and dipole terms contribute recoil corrections of order K^2 to the transition probabilities. The dominant contributions up to order K^2 are thus

$$\begin{aligned} P_{1S-nS} &= \left|\langle\, {}^6\mathrm{He}(1s^2\ {}^1S)\left|1-(Kr)^2/6\right|\, {}^6\mathrm{Li}^+(n\ {}^1S)\rangle\right|^2 \\ &= \left|\langle\, {}^6\mathrm{He}(1s^2\ {}^1S)\,|\ {}^6\mathrm{Li}^+(n\ {}^1S)\rangle\right|^2 \\ &\quad - \frac{K^2}{3}\langle\, {}^6\mathrm{He}(1s^2\ {}^1S)\,|\ {}^6\mathrm{Li}^+(n\ {}^1S)\rangle\langle\, {}^6\mathrm{Li}^+(n\ {}^1S)\left|r^2\right|\, {}^6\mathrm{He}(1s^2\ {}^1S)\rangle \end{aligned} \tag{4}$$

$$P_{1S-nP} = K^2\left|\langle\, {}^6\mathrm{He}(1s^2\ {}^1S)|z|\, {}^6\mathrm{Li}^+(n\ {}^1P)\rangle\right|^2 \tag{5}$$

such that

$$\sum_n (P_{1S-nS} + P_{1S-nP}) = 1 + O(K^4) \tag{6}$$

For brevity, we will write $P_{S-S} = A_{S-S} + K^2 B_{S-S}$ and $P_{S-P} = K^2 B_{S-P}$. The recoil correction is then $K^2(B_{S-S} + B_{S-P})$. As will be seen, the two terms are of opposite sign, and so there is extensive cancellation. After summing over all states and ionization stages, the unitarity condition (6) requires $\sum_n (B_{1S-nS} + B_{1S-nP}) = 0$ [5]. Also, one can see by closure that $\sum_n B_{1S-nP} = \langle (z_1+z_2)^2\rangle = \frac{1}{3}\langle 2r_1^2 + 2r_2^2 - r_{12}^2\rangle$ for S-states. For the ground state of He, the tabulated matrix elements [6] yield $\frac{1}{3}(4\times 1.193\,482\,995 - 2.516\,439\,313) = 0.752\,497\,66$, in agreement with the tables to follow.

We employ Stieltjes imaging techniques [7, 8] in Hylleraas coordinates to represent the infinity of bound states for shake-up processes, and the continuum of scatttering states, including autoionizing ststes, for shake-off processes. In this approach, each pseudostate represents a block of physical scattering states over a narrow range of energies, and especially the additional recoil accompanying the emission of the shake-off electrons.

3 Results

The results of the calculations are presented in the tables. In Table 1, the initial state is assumed to be the ground $1s^2\ {}^1S$ state of helium, and the table shows the transition probabilities into energy bins corresponding to Li^+, Li^{++}, and Li^{3+} respectively. The results are expressed in the form

$$P_{i\to f} = A_{i\to f} + K^2 B_{i\to f} \tag{7}$$

Table 1. Singlet transition probability coefficients A and B from ^{6}He($1s^2\ ^1S$), summed over pseudostate energy bins for ^{6}Li$^+$, ^{6}Li^{++}, and ^{6}Li^{3+}, where $P = A + K^2B$.

Ion	A_{S-S}	A_{S-P}	$A_{\rm Total}$	$A_{\rm Exp't.}$ [5]
Li^+	0.8903(3)	0.0	0.8903(2)	0.899(2)
Li^{++}	0.097(1)	0.0	0.097(1)	0.101(2)
Li^{3+}	0.012(1)	0.0	0.012(1)	0.00018(15)
Total	0.999(1)	0.0	0.999(1)	1.000(2)
Ion	B_{S-S}	B_{S-P}	$B_{\rm Total}$	$B_{\rm Exp't.}$ [5]
Li^+	–0.6650(2)	0.5730(2)	–0.0920(3)	–0.67(11)
Li^{++}	–0.078(2)	0.165(1)	0.087(2)	0.63(11)
Li^{3+}	–0.009(1)	0.014(1)	0.005(2)	0.049(20)
Total	–0.752(2)[1]	0.752(2)[1]	0.000(2)	-0.01(11)

[1] $\mp$0.752 497 66 by closure. See text following Eq. (6).

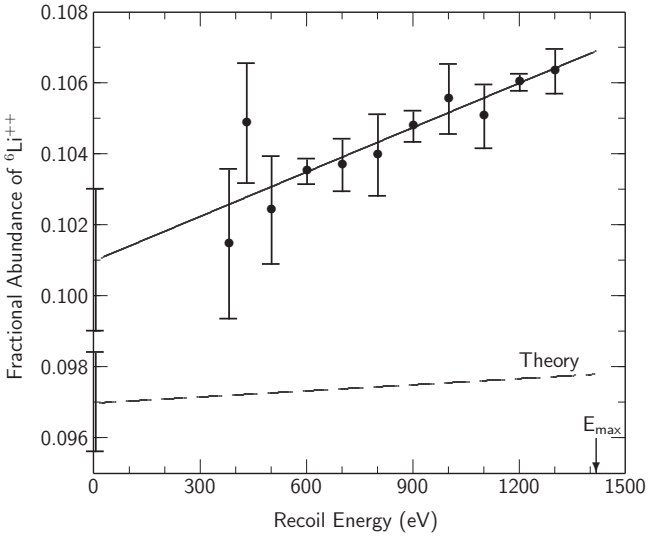

Figure 1. Comparison of theory and experiment for the fractional abundance of ^{6}Li^{++} as a function of recoil energy. The plotted points are from Carlson *et al.* [5], and the solid line is the least-squares fit. The dashed line is the theoretical probability $P(^6\mathrm{Li}^{++}) = A_{S-S} + (B_{S-S} + B_{S-P})K^2$ with $K^2 = E/(149.2 \times 10^3\,\mathrm{eV})$. The maximum recoil energy is $E_{\rm max} = 1418$ eV. The error bars on the vertical axis compare theory and experiment for A_{S-S}.

where $A_{i\to f}$ is the nonrecoil contribution, and $B_{i\to f}$ is the recoil contribution such that $149.2K^2 = E_{\rm rec}$ is the ion recoil energy in keV. The upper part of the table shows that the transition probabilities sum to unity when summed over all ionization states, and the lower part shows that the recoil coefficients $B_{i\to f}$ sum to zero, as expected. It is clear that the $S-P$ recoil term is canceled by the $S-S$ recoil contribution. We present similar results for the case of a He($1s2s\ ^3S$) initial state in Table 2.

Table 2. Triplet transition probability coefficients A and B from ^{6}He($1s2s\ ^3S$), summed over pseudostate energy bins for $^6Li^+$, $^6Li^{++}$, and $^6Li^{3+}$, where $P = A + K^2B$.

Ion	A_{S-S}	A_{S-P}	$A_{\rm Total}$
Li^+	0.88711(3)	0.0	0.88711(3)
Li^{++}	0.0942(7)	0.0	0.0942(7)
Li^{3+}	0.0186(7)	0.0	0.0186(7)
Total	0.9999(7)	0.0	0.9999(7)
Ion	B_{S-S}	B_{S-P}	$B_{\rm Total}$
Li^+	–6.718(0)	6.553(0)	–0.165(0)
Li^{++}	–0.741(7)	0.896(1)	0.155(1)
Li^{3+}	–0.143(7)	0.154(1)	0.011(1)
Total	–7.602(10)	7.603(2)	0.001(2)

In summary, this work provides the first calculations of the recoil term for the ^{6}Li ions formed by the β decay of neutral ^{6}He atoms, and the validity of a sum rule is directly demonstrated. The total result $0.005(1)K^2$ for Li^{3+} is in reasonable accord with the value $0.0000412E_{\rm rec} = 0.00615K^2$ obtained by Couratin *et al.* [9] for the corresponding one-electron $^6He^+$ case. However, the comparison with experiment in Table 1 shows that the calculated recoil contributions are nearly an order of magnitude smaller than the measured values from the experiment of Carlson *et al.* [5]. The disagreement between theory and experiment corresponds to the markedly different slopes in Fig. 2. Since the theoretical results are tightly constrained by the sum rules, it is difficult to see what change could be made to bring theory and experiment into agreement. Renewed experimental work would therefore be of great interest to resolve the disagreement between theory and experiment.

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