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Internal ionization during alpha decay: A new theoretical approach*

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A new theoretical treatment of the problem of orbital-electron ejection during α decay is described. The internal-ionization probability appears as the special zero-impact-parameter trajectory in a generalized impact-parameter formulation of the binary-encounter approximation described recently by the author. The probability of internal ionization during α decay of ^{210}Po is calculated for the $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ subshells in the daughter Pb atom. Markedly improved agreement with experimental results is found.

The problem of orbital-electron ejection during α decay has stubbornly resisted the experimental-theoretical corroboration one should expect, considering the numerous and elaborate calculations and measurements which have been carried out over the years. The original calculation by Migdal,[1] starting from a time-dependent perturbation formulation, has periodically undergone refinements, but these refinements have in general led to even more questionable agreement with experiment than the considerably-less-involved Migdal calculation. In the most recent calculation of this sort, Rubinson[2] reported that the ratios of measured to theoretical ejection probabilities during ^{210}Po α decay for the K, L, and M shells are 15, 270, and 410, respectively. A few years following the Rubinson paper, Ciochetti and Molinari[3] argued that the Migdal approach inherently neglected the monopole interaction, but in Ref. 3 results for the K shell alone were presented, where the agreement appears to be within a factor of 2 of the more recent experimental results.

In the present paper we implement an approach to the calculation of the internal-ionization probability for the K, L, and M shells during ^{210}Po decay which is based upon a model which has recently been described in some detail and applied to a number of problems relevant to ionization and multiple ionization by incident light ions.[4] The model includes the effects of relativity associated with the bound electrons, as well as the diminution of kinetic energy of the α particle owing to its potential energy with respect to the residual nucleus. In the case of the K shell, each of these corrections is very large (>10) and oppositely signed, and may explain in part the failure of all previous calculations, which neglected one or both of these effects. Nuclear recoil effects do not appear to play an important role in the interaction, and the use of (Slater-) screened hydrogenic wave functions leads to theoretical values in reasonable agreement with the most recent experimental results for the K, L, and M shells.

As given in Ref. 4, the ionization probability as a function of impact parameter b for a particle which approaches the atom externally, i.e., charged-particle bombardment, can be written as

$$P(b)=q^2n\int_{-\infty}^{\infty}\sigma\{v_1[(b^2+z^2)^{1/2}],v_2[(b^2+z^2)^{1/2}]\}\times\rho[(b^2+z^2)^{1/2}]\,dz\,, \tag{1}$$

where q is the charge of the incident particle and n the number of electrons in the shell. $\sigma\{v_1[(b^2+z^2)^{1/2}],\, v_2[(b^2+z^2)^{1/2}]\}$ is the cross section for all energy transfers which exceed the binding energy of an electron of initial velocity v_2 located at a distance $(b^2+z^2)^{1/2}$ from the nucleus by a proton of velocity v_1 similarly located. The quantity ρ is the charge density, i.e., the square of the configuration-space wave function. The ionization cross section is found by integrating Eq. (1) (multiplied by $2\pi b$) over all impact parameters b from zero to infinity.

In the present case we are interested only in the limiting expression of Eq. (1) for impact parameter $b=0$, and our integration extends only from $z=0$ to $z=\infty$ since the α particle emerges from the nucleus. Under these conditions, the internal ionization probability is thus

$$P=P(b=0)=4n\int_0^{\infty}\sigma[v_1(z),\,v_2(z)]\rho(z)\,dz\,. \tag{2}$$

The factor 4 preceding the integral arises from squaring the charge (+2) of the α particle. The quantity $\sigma(v_1,\,v_2)$ has been given earlier by Gerjuoy[5] and Vriens,[6] and has been shown to be the result of an exact treatment of the two-body interaction both classically and quantum mechanically, provided the mass of the incident particle is much greater than that of the target (electron).[6] To compute Eq. (2) we must relate the average velocity of the α particle and the electron to their distance from the nucleus. Owing to the repulsive potential of the positively charged nucleus, the kinetic energy of the α particle is diminished at small separations of α particle and nucleus and obeys the following relationship:

$$\tfrac{1}{2}Mv_1^2(r)+(Z_1Z_2e^2/r)=T(\infty), \qquad (3)$$

from which we can immediately derive the necessary $v_1(r)$. $T(\infty)$ in the above expression represents the kinetic energy of the α particle at large distances from the nucleus. The relationship between the bound-electron velocity and its distance from the nucleus has been given in Ref. 4 as the roots of the equation

$$\int_{v'}^{\infty} R_{n,l}^2(v)\,dv-\int_0^{r'} \tilde{R}_{n,l}^2(r)\,dr=0, \qquad (4)$$

where $R_{n,l}(v)$ and $\tilde{R}_{n,l}(r)$ are the solutions to the radial wave equation in momentum space and configuration space, respectively. Equation (4) describes an electron velocity, the magnitude of which decreases monotonically with increased (electron) distance from the nucleus.[7]

Two final questions must be considered in order to carry out the integration indicated by Eq. (2). The first of these questions deals with the effects of recoil of the daughter atom (^{208}Pb); the latter regards the effects of adiabatic rearrangement of the residual Pb atom. Inserting the terminal recoil energy ($\simeq$100 keV) into Eq. (3) for $T(\infty)$, we find that the recoil atom reaches approximately one-half of its terminal kinetic energy at distances of approximately $4a_0/82$ ($1a_0=5.29\times10^{-9}$ cm) and that the recoil energy is negligible for a separation of daughter atom and α particle of less than $2a_0/82$ (where a_0 is the Bohr radius). As a consequence, the effects of recoil will have negligible effect upon the K- and L-shell ionization probabilities and may enhance only slightly the M-shell ionization probability. We have ignored these small effects for all three shells in the present calculation.

Atomic rearrangement of the daughter atom influences our choice of a suitable ionization potential for the bound electrons as well as our choice of appropriate screening coefficients for the atomic wave functions. Ignoring momentarily the effects of Coulomb excitation and ionization by the emerging α particle, the degree of excitation experienced by the residual Pb atom is dependent upon the adiabaticity of the decay. Assuming an instantaneous change from $Z=84$ to $Z=82$ one estimates an average excitation energy of 540 eV.[8] In the present case of near adiabicity ($\simeq$75%) the average excitation due to this effect should be considerably less ($\simeq$150 eV).

Returning to the problem of Coulomb excitation, an extrapolation of the present calculated values, i.e., P versus binding energy, arising from the Coulomb ejection mechanism suggests that only in the case of the $n=5$ or $n=6$ shells should a high degree of excitation occur. This should lead to only a small increase ($\simeq$100 ev) in the total energy, and the combined excitation is thus estimated to be less than 250 eV. This excitation energy constitutes approximately 0.3%, 2%, and 8% of the binding energies of the K, L, and M shells, but must be distributed among a number of ejected electrons; thus it can be assumed to have a negligible effect upon the ionization probability.[9]

As the α particle emerges from the nucleus the electronic charge distribution will attempt to adjust to this new noncentral potential, and the momentum distribution of the electrons will, at the time of the interaction, therefore lie between the momentum distribution of the $Z=84$ atom and the $Z=82$ atom. In order to minimize errors, ionization probabilities have been calculated for the K, L, and M shells assuming the momentum distribution to be that of a Slater-screened $Z=83$ atom. Calculations using $Z=82$ and $Z=84$, respectively, lead to values for the K shell 10% lower and higher, respectively. Similar calculations for the L and M shells indicate that negligible differences arise through alteration by unity of the assumed effective charge of this nucleus.

The present calculated values are compared in Table I with the results of previous calculations. The present results for the K shell are 15-20 times larger than the most refined Migdal calculations by Levinger[10] and Rubinson[2] and are of the same order of magnitude as the results of Ciochetti and Molinari.[3] Neglect, in each of the earlier calculations, of relativistic effects as well as the effects arising from the diminution of kinetic energy of the α particle in the Coulomb field of the nucleus seriously limits objective comparison with the present work. For the case of the L and M shells, the above-mentioned effects are considerably smaller than for the K shell and the present calculations are 200 and 300 times larger than the Rubinson calculation for the L and M shells, respectively. Calculations along the lines described in Ref. 3 would, in the case of the L or M shell, provide a useful test of the suggestion of those authors that the failure of the Migdal-type calculations arose from discarding the monopole interaction.

In Table II the present calculated values of photon yields per α decay for the K, L, and M shells are compared with the existing experimental data. Fluorescence yields from Ref. 11 have been used

TABLE I. Comparison of theoretical internal-ionization probabilities per α decay of ^{210}Po.

Electron shell	Ionization probability per α	Reference
1s	12.5 (−7) [a]	b
	1.0 (−7)	c
	1.42 (−7)	d
	8.7 (−7)	e
	20.2 (−7)	Present
2s	0.53 (−4)	c
	2.30 (−4)	Present
$2p_{1/2}$	0.12 (−4)	c
	0.76 (−4)	Present
$2p_{3/2}$	0.47 (−4)	c
	2.86 (−4)	Present
L_{tot}	1.1 (−4)	c
	0.028 (−4)	d
	5.9 (−4)	Present
3s	17.4 (−4)	Present
3p	56.6 (−4)	Present
3d	116 (−4)	Present
M_{tot}	190 (−4)	Present
	0.556 (−4)	d

[a] The numbers in parentheses represent the powers of ten multiplying the preceding numbers.
[b] Reference 1.
[c] Reference 10.
[d] Reference 2.
[e] Reference 3.

to convert the theoretical ionization probabilities per α decay to photon yields per α decay. In the case of the K shell, the K-fluorescence yield is approximately unity (0.97) and the ionization probability and photon yield are approximately the same. The present calculated values for the K shell agree within the estimated error of all reported measurements, save for the measurement by Ovechkin and Tsenter,[12] which is approximately 75% of the present calculated values.

The calculated L-shell ionization probabilities are related to the L x-ray yields by

$$P_{L_x} = P_{L_1}[\omega_1 + f_{12}\omega_2 + (f_{13} + f_{12}f_{23})\omega_3] + P_{L_2}(\omega_2 + f_{23}\omega_3) + P_{L_3}\omega_3 , \tag{5}$$

P_{L_1}, P_{L_2}, and P_{L_3} being the calculated ionization probabilities. The subshell fluorescence yields, ω_1, ω_2, and ω_3, represent the probability that a vacancy in the subshell designated by the attached subscript emits an x ray characteristic of that subshell. The Coster-Kronig transition probabilities f_{12}, f_{13}, and f_{23} represent the probability that a vacancy initially present in one L subshell (the first subscript) moves to a higher subshell (the second subscript). Average experimental values[11] of 0.07, 0.363, and 0.325 for ω_1, ω_2, and ω_3 and 0.160, 0.580, and 0.156 for f_{12}, f_{13}, and f_{23} were used in the present comparison. The present results are in quite good agreement with the results of Riou,[13] but only constitute approximately 60% of the measured x-ray yield of Rubinson. In the case of the M shell, a mean M-shell fluorescence yield of 0.03 was used,[11] and again the calculated values are approximately 60% of the measured values of Rubinson.

TABLE II. Comparison of present theoretical and measured photon yields from ^{210}Po decay.

Electron shell	Present theoretical yield	Measured yield	Reference
K	1.96 (−6)	1.5 ± 0.5 (−6)	a
		2.0 ± 0.32 (−6)	b
		1.6 ± 0.5 (−6)	c
		1.5 ± 0.4 (−6)	d
L	1.83 (−4)	2.2 ± 0.5 (−4)	c
		2.93 ± 0.43 (−4)	e
		4 (−4)	f
M	0.57 (−3)	1.5 (−3)	f
		0.91 ± 0.13 (−3)	g

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In general, we conclude that the present model yields an adequate treatment of the problem of internal ionization during α decay. Improved wave functions in the case of the L and M shells might have been used in the present calculation, but uncertainties in the L and M shell fluorescence yields inherently set a lower limit to the "errors" in the theoretical photon yields. Solely on the basis of statistical arguments one would surmise that the average fluorescence yields for the L and M shells taken from Ref. 11 are not so large as the corresponding yields in the residual Pb atom, which may have a number of additional electrons missing from the N and O shells.[14] This in principle would tend to bring the theoretical and experimental values in somewhat closer agreement, but increased fluorescence yields of the order of the above-mentioned 60% do not appear likely to occur.

In the case of an instantaneous change in the nuclear charge, the inability of the electrons to adjust to the rapidly varying field can lead to electron "shakeoff." The moderately slow emergence of the α particle permits us to ignore the shakeoff of K, L, or M shell electrons in the present calculations; thus we assume Coulomb ejection to be the sole mechanism by which inner-shell vacancies are created.

In another well-studied area—namely, internal ionization during β (negaton) decay[15]—the conditions of a sudden change are approximated, particularly in the case of high-energy β decay. In this case it is customary to assume that the direct collision mechanism is negligible by comparison with the shakeoff mechanism. The present agreement appears sufficient to warrant a study of those cases in β decay which lie intermediate between the "sudden" and "adiabatic" conditions, through combination of the present theory with those attending exclusively to the shakeoff mechanism.

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[15]Several extensive reviews of this subject are covered in detail in *Proceedings of the International Conference on Inner-Shell Ionization Phenomena and Future Applications, Atlanta, Georgia, 1972,* edited by R. W. Fink, S. T. Manson, J. M. Palms, and P. Venugopala Rao, CONF.-720404 (U. S. AEC, Oak Ridge, Tenn., 1973), Vol. 3.