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Radiative decay rates of metastable one-electron atoms

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Numerical calculations of the $2E1$ and $M1$ decay rates of the $2s_{1/2}$ metastable states of the hydrogen isoelectronic sequence are presented. The $2E1$ rates are found to be in good agreement with recent calculations of Goldman and Drake, but substantially different from the earlier numerical values of Johnson. Effects of nuclear finite size on the $2E1$ rates are found to be insignificant, whereas finite-size effects reduce the $M1$ rate by about 1.1% at $Z=92$.

I. INTRODUCTION

There is continuing interest in accurate calculations of the radiative decay rates of the $2s_{1/2}$ metastable states in hydrogenlike atoms.[1] The largest contributions to these rates are due to the emission of two $E1$ photons (dominant at low Z) and the emission of a single $M1$ photon (dominant at high Z). The $2E1$ rates have been obtained with progressively greater accuracy since the first attempts made at their calculations,[2] while the $M1$ rates are known in closed analytical form.[3]

The most recent calculations of the $2E1$ rates are those of Goldman and Drake.[4] Their calculations, using finite basis sets to represent the Dirac Green's function, have yielded results substantially different from previous direct numerical calculations due to Johnson.[3] Goldman and Drake have pointed out that these discrepancies arise because higher-order terms in the expansion of the photon multipole potential were omitted in Ref. 3. This is confirmed in the present Communication, where the $2E1$ rate is recalculated (treating the multipole potential exactly) by a direct numerical Green's-function technique. Comparison of the results so produced show close agreement with those of Goldman and Drake. The small remaining discrepancies may be attributed to the difference in the methods used to treat the hydrogenic Green's function.

The effects of finite-nuclear size are easily incorporated into the present calculation. These effects have been investigated and are found to be marginal for $2E1$ decay. Finite-nuclear-size modifications of the $M1$ rates are also calculated numerically and are found to produce larger changes in the $M1$ rates than in the $2E1$ rates.

II. CALCULATION OF THE DECAY RATES

The two-photon decay rate for low Z in one-electron ions is dominated by the $2E1$ decay mode. The corresponding decay probability per unit time may be expressed in differential form as

$$\frac{dw}{d\omega_1}=\frac{8}{27\pi}\alpha^2\omega_1^3\omega_2^3\{\tfrac{1}{3}[E_1^2(\omega_1,\omega_2)+E_1^2(\omega_2,\omega_1)]+\tfrac{2}{3}[E_{-2}^3(\omega_1,\omega_2)+E_{-2}^2(\omega_2,\omega_1)]$$
$$-\tfrac{2}{9}E_1(\omega_1,\omega_2)E_1(\omega_2,\omega_1)+\tfrac{8}{9}[E_{-2}(\omega_1,\omega_2)E_1(\omega_2,\omega_1)+E_1(\omega_1,\omega_2)E_{-2}(\omega_2,\omega_1)]\}\ , \quad (1)$$

where ω_1 and ω_2 are the energies of the two photons in natural units. In Eq. (1) the transition amplitude $E_\kappa(\omega_1,\omega_2)$ is given by

$$E_\kappa(\omega_1,\omega_2)=\frac{3}{\omega_2}\int_0^\infty dr\,[S_\kappa(r,\omega_1)U_\kappa(r,\omega_2)+T_\kappa(r,\omega_1)V_\kappa(r,\omega_2)]\ , \quad (2)$$

where S_κ and T_κ are solutions of the perturbed Dirac equation

$$(m-\epsilon_1+\omega_1-V)S_\kappa(r,\omega_1)+\left(\frac{d}{dr}-\frac{\kappa}{r}\right)T_\kappa(r,\omega_1)=\frac{3}{\omega_1}K_\kappa(r,\omega_1)\ ,$$
$$-\left(\frac{d}{dr}+\frac{\kappa}{r}\right)S_\kappa(r,\omega_1)-(m+\epsilon_1-\omega_1-V)T_\kappa(r,\omega_1)=\frac{3}{\omega_1}\,L_\kappa(r,\omega_1) \quad (3)$$

for $\kappa = 1, -2$.

Equations (3) are solved using a numerically constructed Green's function. The resulting values of the decay rate are obtained by numerical integration of Eq. (2) to obtain the reduced transition amplitude $E_\kappa(\omega_1, \omega_2)$. The present calculation is carried out using two gauges for the photon field: the Coulomb gauge (which leads in the nonrelativistic limit to velocity-form transition amplitudes), and the length[5] gauge (which leads in the same limit to length-form amplitudes). The use of two gauges serves as a check on the consistency of the numerical procedure since the calculation is, in principle, gauge invariant.

The inhomogeneous terms K_κ, L_κ in Eq. (3) and the terms U_κ and V_κ in the integrand of Eq. (2) are different in each gauge:

$$K_\kappa(r,\omega_1) = \begin{cases} \dfrac{\kappa+1}{2}\left[j_1'(\omega_1 r) + \dfrac{j_1(\omega_1 r)}{\omega_1 r}\right] F_{2s_{1/2}}(r) - \dfrac{j_1(\omega_1 r)}{\omega_1 r} F_{2s_{1/2}}(r) & \text{(Coulomb gauge)} \\ j_1(\omega_1 r) G_{2s_{1/2}}(r) - \left[\dfrac{\kappa+1}{2} + 1\right] j_2(\omega_1 r) F_{2s_{1/2}}(r) & \text{(length gauge)} \,, \end{cases} \tag{4a}$$

$$L_\kappa(r,\omega_1) = \begin{cases} \dfrac{\kappa+1}{2}\left[j_1'(\omega_1 r) + \dfrac{j_1(\omega_1 r)}{\omega_1 r}\right] G_{2s_{1/2}}(r) - \dfrac{j_1(\omega_1 r)}{\omega_1 r} G_{2s_{1/2}}(r) & \text{(Coulomb gauge)} \\ j_1(\omega_1 r) F_{2s_{1/2}}(r) - \left[\dfrac{\kappa+1}{2} + 1\right] j_2(\omega_1 r) G_{2s_{1/2}}(r) & \text{(length gauge)} \,, \end{cases} \tag{4b}$$

$$U_\kappa(r,\omega_2) = \begin{cases} \dfrac{-(\kappa+1)}{2}\left[j_1'(\omega_2 r) + \dfrac{j_1(\omega_2 r)}{\omega_2 r}\right] F_{1s_{1/2}}(r) + \dfrac{j_1(\omega_2 r)}{\omega_2 r} F_{1s_{1/2}}(r) & \text{(Coulomb gauge)} \\ j_1(\omega_2 r) G_{1s_{1/2}}(r) + \left[\dfrac{\kappa+1}{2} + 1\right] j_2(\omega_2 r) F_{1s_{1/2}} & \text{(length gauge)} \,, \end{cases} \tag{5a}$$

$$V_\kappa(r,\omega_2) = \begin{cases} \dfrac{-(\kappa+1)}{2}\left[j_1'(\omega_2 r) + \dfrac{j_1(\omega_2 r)}{\omega_2 r}\right] G_{1s_{1/2}}(r) - \dfrac{j_1(\omega_2 r)}{\omega_2 r} G_{1s_{1/2}}(r) & \text{(Coulomb gauge)} \\ j_1(\omega_2 r) F_{1s_{1/2}}(r) + \left[\dfrac{\kappa+1}{2} - 1\right] j_2(\omega_2 r) G_{1s_{1/2}}(r) & \text{(length gauge)} \,. \end{cases} \tag{5b}$$

Here $j_1(\omega r)$ and $j_2(\omega r)$ are spherical Bessel functions of order 1 and 2, respectively, and $G_{nlj}(r)$ and $F_{nlj}(r)$ are large- and small-component radial Dirac eigenfunctions.

The $M1$ decay rate is given by

$$w(M_1) = \tfrac{4}{9}\alpha\omega^3 |M(\omega)|^2 \,, \tag{6}$$

where

$$M(\omega) = \frac{3}{\omega}\int_0^\infty j_1(\omega r)[G_{1s_{1/2}}(r)F_{2s_{1/2}}(r) + G_{2s_{1/2}}(r)F_{1s_{1/2}}(r)]dr \,. \tag{7}$$

When a spherically symmetric nucleus of finite extension is used, the Coulomb potential in the radial Dirac equations is replaced by the potential due to the Fermi charge distribution[6]

$$\rho(r) = \rho_0\{1 + \exp[(r-c)/a]\}^{-1} \,, \tag{8}$$

where $c = (1.183A^{1/3} - 0.353)$ fm and $a = 0.52$ fm, and the Dirac-Coulomb functions by their numerically generated counterparts.

As has been shown by Lin and Feinberg[7] and by Barbieri and Sucher,[8] radiative corrections have no effect to lowest order in αZ on the $M1$ matrix element. Thus the effect of radiative corrections is simply to modify the factor ω in Eq. (6) to incorporate the effects of radiative corrections.

III. RESULTS

In Table I we compare the $2E1$ rates from the present numerical evaluation of Eqs. (1)–(3) with

TABLE I. Coulomb field $2E1$ decay rates in $\sec^{-1}$. Z is the nuclear charge.

Z	$Z^{-6}w(2E1)$ Goldman and Drake[a]	$Z^{-6}w(2E1)$ This calculation
1	8.2291	8.2291
20	8.1181	8.1196
40	7.8096	7.8116
60	7.3446	7.3453
80	6.7440	6.7426
92	6.3097	6.3093

[a] S. P. Goldman and G. W. F. Drake, Ref. 4.

the calculations of Goldman and Drake. We believe that the present calculations are accurate to all figures quoted, as agreement between length- and velocity-gauge values continues to at least two figures beyond those shown in the table.

The effects of finite-nuclear size on the $2E1$ rates are illustrated in Table II. These effects are seen to be extremely small. For example, at $Z=92$, we find from Table II,

$$Z^{-6}w(2E1)=\begin{cases}6.3093 & \text{point nucleus}\\ 6.3084 & \text{finite nucleus}\ .\end{cases}$$

In Table III we show the corresponding modification of the $M1$ rate which results when we use finite-nucleus wave functions. We see that the $M1$ rate decreases by about 1.1% for $Z=92$.

Our final values for the $2s_{1/2}$ decay rates are given in Table IV. In column 3 of this table we list the $M1$ rate including finite-nucleus-size effects. The $2E1$ rates also include the very small corrections due to finite-nuclear size. In the final column of Table IV we give the total rates determined by adding to the $2E1$ and $M1$ rates the small corrections due to the $2M1$, $E1M2$, and other decay modes.[4] The final

TABLE II. Comparison of Coulomb-field decay rates with those calculated using a Fermi field. Rates are in $\sec^{-1}$. Z is the nuclear charge. A is the nucleon number.

Z	A	$Z^{-6}w(2E1)$ Point nucleus	$Z^{-6}w(2E1)$ Finite nucleus
1	1	8.2291	8.2291
20	40	8.1196	8.1196
40	90	7.8116	7.8114
60	142	7.3453	7.3447
80	202	6.7426	6.7412
92	238	6.3093	6.3084

TABLE III. Comparison of $M1$ decay rates calculated using a point-nucleus field and the field due to a finite-nuclear-charge distribution. Rates are in $\sec^{-1}$. Z is the nuclear charge. A is the nucleon number.

Z	A	$10^6Z^{-10}w(M1)$ Point nucleus	$10^6Z^{-10}w(M1)$ Finite nucleus
1	1	2.4959	2.4958
20	40	2.5537	2.5536
40	90	2.7415	2.7410
60	142	3.1114	3.1084
80	202	3.7939	3.7768
92	238	4.4817	4.4310

TABLE IV. Metastable state decay rates including finite-nuclear-size effects. Decay rates are in $\sec^{-1}$. Z is the nuclear charge. A is the nucleon number. w(tot) is written $a(b)$. This is to be interpreted as $a\times 10^{b}$.

Z	A	10^6Z^{-10} $w(M1)$	Z^{-6} $w(2E1)$	w(tot)
1	1	2.4958	8.2291	8.2291 (00)
2	4	2.4963	8.2282	5.2661 (02)
3	7	2.4970	8.2268	5.9975 (03)
4	9	2.4980	8.2249	3.3692 (04)
5	11	2.4993	8.2223	1.2850 (05)
6	12	2.5009	8.2193	3.8363 (05)
7	14	2.5027	8.2157	9.6727 (05)
8	16	2.5049	8.2115	2.1553 (06)
9	19	2.5073	8.2068	4.3702 (06)
10	20	2.5100	8.2015	8.2266 (06)
12	24	2.5163	8.1893	2.4609 (07)
14	28	2.5238	8.1750	6.2284 (07)
16	32	2.5325	8.1586	1.3966 (08)
18	36	2.5424	8.1401	2.8594 (08)
20	40	2.5536	8.1196	5.4580 (08)
22	48	2.5660	8.0970	9.8620 (08)
24	52	2.5797	8.0725	1.7063 (09)
26	56	2.5948	8.0461	2.8519 (09)
28	58	2.6112	8.0179	4.6372 (09)
30	64	2.6290	7.9878	7.3756 (09)
34	80	2.6691	7.9223	1.7749 (10)
38	88	2.7154	7.8500	4.0685 (10)
42	98	2.7684	7.7713	8.9946 (10)
46	106	2.8287	7.6865	1.9283 (11)
50	120	2.8969	7.5958	4.0161 (11)
54	132	2.9740	7.4995	8.1302 (11)
58	140	3.0609	7.3976	1.6004 (12)
62	152	3.1586	7.2904	3.0654 (12)
66	164	3.2687	7.1779	5.7200 (12)
70	174	3.3926	7.0600	1.0415 (13)
74	184	3.5324	6.9367	1.8534 (13)
78	195	3.6903	6.8078	3.2296 (13)
82	208	3.8690	6.6731	5.5210 (13)
86	222	4.0719	6.5322	9.2759 (13)
90	232	4.3033	6.3848	1.5345 (14)
92	238	4.4310	6.3084	1.9631 (14)

column is based on the value $R = 1.097\,373\,1 \times 10^5$ cm^{-1}. Reduced mass corrections have not been included in Table IV; these corrections may be easily incorporated by multiplying the entries by the ratio $1/(1+m/M)$ where m is the mass of the electron and M that of the nucleus.

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