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Accurate values of the Lamb shift can be derived from measurements of the anisotropy in the angular distribution of the radiation accompanying the electric field induced $2s$-$1s$ transition of hydrogen. Calculations of the anisotropy, including relativistic and hyperfine structure corrections, are presented for the hydrogenic ions up to S^{15+}. The data enable the calculation of the Lamb shift from a measured value of the anisotropy.

INTRODUCTION

There has been much recent interest, both experimental[1,2] and theoretical,[3,4] in the Lamb shifts of heavy hydrogenic systems. In previous papers,[5,6] we have suggested that measurements of the angular anisotropy in the electric field quenching radiation from the metastable $2s_{1/2}$ state may provide an accurate method of deriving the Lamb shifts of hydrogenic ions. A nonperturbative theory of the process has been developed[7] and the technique has been tested to high precision in hydrogen and deuterium.[8]

For hydrogenic ions with nuclear charge Z greater than five or six, first-order perturbation theory is adequate for readily obtainable electric quenching fields (i.e., fields up to about $50Z^4$ V/cm). Under these conditions, the anisotropy is very nearly equal to its zero-field value, and therefore independent of field strength. In this paper, we present calculations of the zero-field anisotropies as a function of the Lamb shift for the ions up to hydrogenic sulphur. Lamb shifts can then be derived when experimental measurements of the anisotropy are available. The calculations include nuclear-spin and relativistic effects.

THEORY

The theory presented previously[7,8] is modified here to include relativistic corrections in the evaluation of the transition matrix elements. The calculations are performed in the coupled representation $\vec{F}=\vec{j}+\vec{I}$, where $\vec{j}$ is the total electronic angular momentum and $\vec{I}$ is the nuclear spin. We assume that the metastable ion beam is initially an incoherent mixture of all the hyperfine states of the $2s_{1/2}$ level with equal statistical weights. Then in the limit of weak-field strength $\mathcal{F}$, the induced electric dipole transition rate can be written in the form

$$I(\hat{e})=\frac{2\pi}{\hbar}\frac{\rho(\bar{\omega})}{(2I+1)(2j+1)}\times(|\hat{e}\cdot\hat{F}|^2|A|^2+|\hat{e}\times\hat{F}|^2|A'|^2), \tag{1}$$

where $\rho(\bar{\omega})$ is the density of photon states at the average emitted frequency $\bar{\omega}$, $\hat{e}$ is the photon polarization vector, and $\hat{F}$ is a unit vector pointing in the electric field direction. The coefficients A and A' correspond to transitions in which $\Delta M=0$ and ±1, respectively. $|A|^2$ is given by (in atomic units)

$$|A|^2=\sum_{F,M,F'}\left|\sum_{j''F''}\langle 1s,\,F'M'|\vec{\alpha}\cdot\vec{\mathfrak{A}}|2p,\,j''F''M\rangle\times\frac{\langle 2p,\,j''F''M|\mathcal{F}z|2s,\,FM\rangle}{E(2p,\,j''F'')-E(2s,\,F)}\right|^2 \tag{2}$$

with $M'=M$. Here, $\vec{\alpha}$ is the 4×4 Dirac matrix and $\vec{\mathfrak{A}}$ is the electric dipole vector potential for the emitted photon. The corresponding expression for $|A'|^2$ is the same except that $M'=M\pm1$.

For electric dipole transitions, the relativistic matrix elements in Eq. (2) are both of the form $\langle\gamma'j'IF'M'|T(1q)|\gamma jIFM\rangle$, where $T(1)$ is an irreducible tensor of rank 1. Using standard vector coupling techniques, the matrix elements can be written in terms of 3-j and 6-j symbols as

$$\langle\gamma'j'IF'M'|T(1q)|\gamma jIFM\rangle=(-1)^{F'-M'}\begin{pmatrix}F' & 1 & F\\ -M' & q & M\end{pmatrix}\times(-1)^{j'+I+F+1}[(2F+1)(2F'+1)]^{1/2}\times\begin{Bmatrix}j' & F' & I\\ F & j & 1\end{Bmatrix}\langle\gamma'j'\|T(1)\|\gamma j\rangle. \tag{3}$$

Following Grant,[9] the reduced matrix elements are

$$\langle \gamma' j' \| T(1) \| \gamma j \rangle = (-1)^{j'-1/2}[(2j'+1)(2j+1)]^{1/2} \times \begin{pmatrix} j' & 1 & j \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{pmatrix} \bar{M}_{j',j}, \quad (4)$$

where in the Coulomb gauge

$$\bar{M}_{j',j} = i(\omega/\pi c)^{1/2}\{(2)^{-1/2}[(\kappa' - \kappa)I_2^+ + 2I_2^-] - (2)^{1/2}[(\kappa' - \kappa)I_0^+ - I_0^-]\} \quad (5)$$

for the $\vec{\alpha} \cdot \vec{\alpha}$ matrix element, and

$$\bar{M}_{j',j} = \mathfrak{F} \int_0^\infty (P'P + Q'Q) r \, dr \quad (6)$$

for the $\mathfrak{F}z$ matrix element. In the above,

$$I_L^\pm = \int_0^\infty (P'Q \pm Q'P) j_L(\omega r/c) \, dr; \quad (7)$$

$j_L(x)$ is the spherical Bessel function, and P and Q are the large and small components of the relativistic radial wave functions.[10] The integrals $I_L^\pm$ were calculated analytically by expanding $j_L(\omega r/c)$ and retaining all terms up to $(\omega r/c)^2$.

The quantity of interest in anisotropy measurements is the total intensity summed over both polarizations emitted in directions parallel and perpendicular to the electric field. Summing Eq. (1) over two perpendicular vectors $\hat{e}$, both perpendicular to the direction of propagation, yields

$$I(\theta, \varphi) = \frac{2\pi}{\hbar} \frac{\rho(\bar{\omega})}{(2I+1)(2j+1)}[|A|^2(1 - \cos^2\theta) + |A'|^2(1 + \cos^2\theta)], \quad (8)$$

where θ and φ are the spherical angles defining the direction of propagation and $\hat{F}$ is taken to point in the z direction.[11] The anisotropy R is defined to be

$$R = (I_\parallel - I_\perp)/(I_\parallel + I_\perp), \quad (9)$$

where $I_\parallel = I(0, 0)$ and $I_\perp = I(\frac{1}{2}\pi, 0)$. Thus from Eq. (8)

$$R = (|A'|^2 - |A|^2)/(3|A'|^2 + |A|^2). \quad (10)$$

The calculated values of R are presented in the following section.

RESULTS

In addition to the relativistic matrix elements described in the preceding section, we also need the energy differences in the denominator of Eq. (2), including hyperfine structure. The calculated anisotropies are parametrized in terms of the Lamb shift $S = E(2s_{1/2}) - E(2p_{1/2})$ uncorrected for hyperfine structure. The fine-structure splitting $E(2p_{3/2}) - E(2p_{1/2})$, which to a first approximation is a non-QED effect, can be estimated to sufficient accuracy from the formula[12]

$$E(2p_{3/2}) - E(2p_{1/2}) = \frac{\mathcal{R}_\infty (Z\alpha)^2}{16}\left[[1 + \tfrac{5}{8}(Z\alpha)^2]\left(1 - \frac{m}{M}\right) + \frac{\alpha}{\pi}\left(1 - 2\frac{m}{M}\right) + 2\frac{\alpha}{\pi}(Z\alpha)^2 \ln Z\alpha\right], \quad (11)$$

TABLE I. Input data for the calculation of quenching anisotropies in hydrogenic ions.

Ion	$E(2p_{3/2}) - E(2p_{1/2})$ (Hz)	$\Gamma(2p_{1/2})$ ($\sec^{-1}$)	$\Gamma(2p_{3/2})$ ($\sec^{-1}$)	α_{hfs} [a] (Hz)
^{1}H	1.096 91 (10) [b]	6.2683 (8)	6.2682 (8)	2.6635 (8)
^{2}H	1.097 21 (10)	6.2683 (8)	6.2682 (8)	4.0923 (7)
^{4}He	1.755 94 (11)	1.0030 (10)	1.0029 (10)	0
^{7}Li	8.891 41 (11)	5.0776 (10)	5.0768 (10)	2.7960 (9)
^{9}Be	2.810 81 (12)	1.6048 (11)	1.6044 (11)	−3.5949 (9)
^{11}B	6.864 41 (12)	3.9183 (11)	3.9165 (11)	1.0686 (10)
^{12}C	1.423 92 (13)	8.1256 (11)	8.1201 (11)	0
^{14}N	2.639 12 (13)	1.5055 (12)	1.5041 (12)	6.6021 (9)
^{16}O	4.504 44 (13)	2.5685 (12)	2.5655 (12)	0
^{19}F	7.219 28 (13)	4.1147 (12)	4.1085 (12)	1.8274 (11)
^{20}Ne	1.101 01 (14)	6.2723 (12)	6.2606 (12)	0
^{23}Na	1.613 10 (14)	9.1844 (12)	9.1637 (12)	9.3811 (10)
^{24}Mg	2.286 35 (14)	1.3010 (13)	1.2975 (13)	0
^{27}Al	3.151 71 (14)	1.7922 (13)	1.7866 (13)	1.5254 (11)
^{28}Si	4.242 94 (14)	2.4110 (13)	2.4022 (13)	0
^{31}P	5.596 68 (14)	3.1778 (13)	3.1645 (13)	3.6404 (11)
^{32}S	7.252 43 (14)	4.1146 (13)	4.0950 (13)	0

[a] *Handbook of Chemistry and Physics*, 52nd ed. (Chemical Rubber Co., Cleveland, 1971), p. E-57.

[b] The numbers in parentheses are the powers of ten by which the entries are to be multiplied.

TABLE II. Data for obtaining the Lamb shift S [Eq. (13)] from a measured value of the anisotropy R.

Ion	S_0 (GHz)	R_0	b
^{1}H	1.057 867 (0)	0.139 071	1.0187
^{2}H	1.059 241 (0)	0.141 165	1.0525
^{4}He	1.404 205 (1)	0.117 966	1.0352
^{7}Li	6.273 75 (1)	0.104 251	1.0218
^{9}Be	1.797 91 (2)	0.094 905	1.0207
^{11}B	4.045 7 (2)	0.087 537	1.0160
^{12}C	7.819 9 (2)	0.081 723	1.0150
^{14}N	1.361 37 (3)	0.076 829	1.0130
^{16}O	2.196 21 (3)	0.072 670	1.0114
^{19}F	3.343 1 (3)	0.069 015	1.0088
^{20}Ne	4.861 1 (3)	0.065 876	1.0091
^{23}Na	6.809 0 (3)	0.062 994	1.0077
^{24}Mg	9.256 0 (3)	0.060 451	1.0074
^{27}Al	1.226 5 (4)	0.058 104	1.0059
^{28}Si	1.590 7 (4)	0.056 016	1.0061
^{31}P	2.025 4 (4)	0.054 082	1.0055
^{32}S	2.537 3 (4)	0.052 299	1.0051

where m/M is the electron-to-nuclear mass ratio, α is the fine-structure constant 1/137.036, and $\mathcal{R}_\infty$ is the Rydberg constant. The hyperfine structure energy shifts are estimated from

$$\Delta E_{nljIF} = \frac{\alpha_{\rm hfs}}{n^3}\left(\frac{F(F+1)-j(j+1)-I(I+1)}{j(j+1)(l+\frac{1}{2})}\right), \quad (12)$$

where $\alpha_{\rm hfs}$ is the hyperfine structure coupling constant. The various input data are listed in Table I.

The Lamb shift corresponding to a measured value of the anisotropy can be obtained from the data in Table II. The dependence of the Lamb shift[5] on the measured anisotropy at zero-field strength is expanded in the form

$$S = S_0[1 + b(R - R_0)/R_0], \quad (13)$$

up to terms linear in $R - R_0$, where S_0 is the theoretical Lamb shift tabulated by Mohr,[4] and R_0 is the corresponding theoretical anisotropy. The values of S_0, R_0, and b are listed in Table II. The error introduced in S by neglecting quadratic and higher terms in $R - R_0$ is less than 0.01% provided that R differs from R_0 by less than 1%. It is clear from the values of b that the fractional change in S from S_0 is nearly equal to the fractional deviation of R from R_0. Although relativistic corrections to the transition integrals have a substantial effect on the values of $|A|^2$ and $|A'|^2$ separately for large Z, their ratio, and therefore the values of R, are nearly unchanged. For hydrogenic sulphur ($Z = 16$), relativistic corrections increase R by only 0.04%.

The values of R_0 for ^{1}H and ^{2}H in Table II are slightly different from the values calculated previously[8] in the limit of zero-field strength owing to the use of the revised Lamb shifts calculated recently by Mohr.[4] There is a further small error in the R_0 for ^{2}H in Ref. 8 in the limit $\mathcal{F} \to 0$ due to the use of an incorrect value for $\alpha_{\rm hfs}$. Using the corrected value $R_0 = 0.141\,165$ yields the experimental Lamb shift $S = 1059.6 \pm 1.1$ MHz instead of the value 1058.7 ± 1.1 MHz given previously from the measured value $R = 0.141\,21 \pm 0.000\,14$. Further experiments are in preparation to extend these measurements to the hydrogenic ions such as O^{7+} and F^{8+}. There does not appear to be any fundamental difficulty which would prevent the attainment of at least the ±0.1% accuracy already demonstrated in neutral hydrogen.[8] This would be a substantial improvement over the accuracy of existing Lamb-shift measurements[2,13-15] for the heavier hydrogenic ions.

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