The Nuclear Moment of Tl

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(Received April 27, 1934)

The value of $\psi^2(0)$ for the $7s$ state of Tl I is calculated relativistically and compared with the value determined from the formula $\psi^2(0)=Z_i Z_0^2/\pi a_H^3 n_0^3$. With the experimental value of the hyperfine structure splitting of this level, the magnetic moment of the Tl nucleus is found to be: $1840g \leqq 2.7$. The f values corresponding to the transitions $p_{3/2}s_{1/2}$ and $p_{1/2}s_{1/2}$ are also determined and are found to be in agreement with experiment when the effect of a perturbation is taken into account.

INTRODUCTION

IN order to calculate nuclear magnetic moments from the hyperfine structure splittings of s levels, one needs the value of $\psi^2(0)$, the probability of finding the s electron in a unit volume near the nucleus. For this calculation, various writers[1, 2, 3] have used the formula $\psi^2(0)=Z_i Z_0^2/\pi a_H^3 n_0^3$ where Z_i is the effective nuclear charge in the inner part of the orbit, a_H the Bohr radius, Z_0 the effective charge in the outer part of the orbit, and n_0 the effective quantum number, defined by equating the term value energy to $-RZ_0^2/n_0^2$. An accurate numerical calculation of $\psi^2(0)$ provides a test for the validity of this semi-empirical formula. The results of several such calculations were reported in reference 2; in some of these the agreement with the formula was good, but in other cases poor. It seemed worth while therefore, to carry out some further calculations.

THEORY

The $7s$ state of Tl I with the term energy 22,787 cm^{-1} was used. The method followed has been outlined by Breit[4] and will be discussed only briefly here. Radial functions closely related to Gordon's F and G are used, and the equations they satisfy are:

$$d\phi_1/dr - j'\phi_1/r = [(2\pi/\Lambda)(1-E/mc^2)+V]\phi_2,$$

$$d\phi_2/dr + j'\phi_2/r = [(2\pi/\Lambda)(1+E/mc^2)-V]\phi_1,$$

$\Lambda=h/mc$, E is the energy, V the potential energy, and for s terms $j'=-1$. The solutions of these equations are used to evaluate

$$\psi^2(0) = -\frac{2}{\Lambda}\frac{\int_0^\infty(\phi_1\phi_2/r^2)dr}{\int_0^\infty(\phi_1^2+\phi_2^2)dr}.$$

With the Fermi-Thomas field for small values of $r(r<0.06a_H)$ solutions may be obtained in terms of hypergeometric functions, and these suffice for calculating $\int_0^\infty(\phi_1\phi_2/r^2)dr$ since the integrand falls off very rapidly with r. The calculation of the normalization integral $\int_0^\infty(\phi_1^2+\phi_2^2)dr$ is simplified by the fact that ϕ_1^2 may be neglected in comparison with ϕ_2^2 throughout the whole range of r which contributes to the integral.

A solution for $\phi_2(r>0.06a_H)$ is obtained by using the Wentzel-Kramers-Brillouin method in a slightly modified form. This leads to a sinusoidal solution which may be joined to the hypergeometric series solution at the first node, and an exponential solution for large r. The sine and exponential solutions do not join, but the gap may be bridged by using the Schroedinger ψ function, since for large values of r, ϕ_2 behaves as $r\psi$. By making a slight change in the field it was possible to join the Schroedinger solution to the sinusoidal W. K. B. solution at its last node. The exponential solution for large values of r was then seen to be identical with the Schroedinger solution in that region.

[1] Pauling and Goudsmit, *Structure of Line Spectra.*
[2] G. Breit, Phys. Rev. **42**, 348 (1932).
[3] McLennan, McLay and Crawford, Proc. Roy. Soc. **A133**, 652 (1931). For modifications of formula see Fermi and Segrè, Zeits. f. Physik **82**, 729 (1933).
[4] G. Breit, Phys. Rev. **38**, 463 (1931).

The Fermi-Thomas field was first changed so that the phase integral was 5.75π in accordance with Kramers' rule. This was accomplished by making the field purely Coulomb beyond a point $r=r_0$, this point being determined by trial. In order to remove the resulting discontinuity in the potential at r_0, the difference between the Fermi-Thomas and Coulomb values at r_0 was subtracted from all values between r_0 and the origin. This process still leaves a break in the slope of the potential function at r_0 which may be smoothed out graphically. No reasonable smoothing out of this break made any difference in the calculations considered. In the final field used, the value of the phase integral had to be increased slightly (about 1 percent) over the value 5.75π. A comparison of this field with that used by Breit[4] showed the two to be practically identical. Thus the same field is in agreement with the experimentally determined energies of $p_{3/2}$, $p_{1/2}$, $s_{1/2}$ states.

The result of this relativistic calculation is $\psi^2(0)=3.7(8)\times10^{25}$ cm^{-3}. The value from the formula $\psi^2(0)=Z_iZ_0^2/\pi a^3{}_H n_0^3$ is 1.7×10^{25} cm^{-3} but the relativity correction must still be applied to this. According to Racah[5] this correction factor is 2.31, so that $\psi^2_{rel.}(0)=3.9\times10^{25}$ cm^{-3}.

The agreement between these two results is as good as could be expected. It is difficult to determine the probable error of this calculation; 10 percent is a rough estimate. Racah has also calculated $\psi^2(0)$ for this state, obtaining a value 11.3×10^{25} cm^{-3}, which is three times as large as that found here.

Calculation of f Values

Knowing the values of ϕ_2 for $p_{3/2}$, $p_{1/2}$, $s_{1/2}$ states, one can calculate the f values for the transitions $p_{3/2}$, $s_{1/2}$ and $p_{1/2}$, $s_{1/2}$ which we denote by f_{5350} and f_{3776}. The f values are given by

$$f_{ji}=(8\pi^2m\nu_{ji}/3h)\sum(m_j)\{|x_{m_j,\,m_i}|^2+|y_{m_j,\,m_i}|^2+|z_{m_j,\,m_i}|^2\}.$$

For the calculation of matrix elements $x_{m_j,\,m_i}$ etc., only the radial function ϕ_2 is used, but the angular dependence must be taken into account. This calculation gives $f_{5350}=0.146$; $f_{3776}=0.114$ as compared with the measured[6,7] values 0.076 and 0.08, respectively.

These discrepancies may be explained by the presence of a perturbing configuration. According to Fermi and Segrè[8] the configuration $6s^26p$ which gives rise to the p terms discussed above is perturbed by the configuration $6s6p7s$ which lies about 7 volts above it. They find that they may use

$$\psi=0.96\psi_0-0.22\psi_1+0.18\psi_2+0.03\psi_3,$$

where ψ is the perturbed eigenfunction for the state $(p_{3/2})_{3/2}$ and

$$\psi_0=\{6s\ S_{1/2},\ 6s\ S_{-1/2},\ (6p)_1\ S_{1/2}\},$$
$$\psi_1=\{6s\ S_{-1/2},\ 7s\ S_{1/2},\ (6p)_1\ S_{1/2}\},$$
$$\psi_2=\{6s\ S_{1/2},\ 7s\ S_{-1/2},\ (6p)_1\ S_{1/2}\},$$
$$\psi_3=\{6s\ S_{1/2},\ 7s\ S_{1/2},\ (6p)_1\ S_{-1/2}\}.$$

These functions are supposed to be antisymmetrized by writing them as determinants with the proper normalization factor.

In order to investigate the effect of this perturbation on f_{5350}, approximate values of ϕ_2 for the $6s$ electron were obtained. The field used was the same as that for the $7s$ electron, and the energy for $6s$ was determined to fit this field. Since no experimental energy for $6s$ was available, this seemed to be the best procedure to adopt. The $7s$ term used in this calculation arises from $6s^27s$ and we represent $(s_{1/2})_{1/2}$ by $\{6s\ S_{1/2},\ 6s\ S_{-1/2},\ 7s\ S_{1/2}\}$. Since the angular dependence for all s terms is the same, the effect of this perturbation is to change only integrals over the radial variable. The perturbation reduces the value of f_{5350} to 0.073, which agrees with the measured value, 0.076 better than could be expected from the accuracy of the calculation.

This perturbation also affects the value of f_{3776} which involves the $p_{1/2}$ state. We represent the unperturbed wave function for $(p_{1/2})_{1/2}$ by

$$(3)^{-\frac{1}{2}}(\phi_0'-(2)^{\frac{1}{2}}\phi_0''),$$

where

$$\phi_0'=\{6s\ S_{1/2},\ 6s\ S_{-1/2},\ (6p)_0\ S_{1/2}\},$$
$$\phi_0''=\{6s\ S_{1/2},\ 6s\ S_{-1/2},\ (6p)_1\ S_{-1/2}\}.$$

[5] G. Racah, Zeits. f. Physik **71**, 431 (1931).

[6] Det. Kgl. Danske Videnskab. Selskab. Mathem. Meddeleser **7**, 12 (1926).

[7] Prokofjew and Solovjev, Zeits. f. Physik **48**, 276 (1928).

[8] Fermi and Segrè, Reale Accademia D'Italia **IV**, 131 (1933).

The radial integrals involved in the calculation of the coefficients for the perturbed $(p_{1/2})_{1/2}$ function, which we denote by ϕ, can be reduced to those evaluated by Fermi and Segrè, and

$$\phi=0.97\phi_0+0.13\phi_1-0.11\phi_2-0.15\phi_3+0.09\phi_4,$$

where

$$\phi_1=\{6s\ S_{-1/2},\ 7s\ S_{1/2},\ (6p)_1\ S_{-1/2}\},$$

$$\phi_2=\{6s\ S_{-1/2},\ 7s\ S_{1/2},\ (6p)_0\ S_{1/2}\},$$

$$\phi_3=\{6s\ S_{1/2},\ 7s\ S_{-1/2},\ (6p)_1\ S_{-1/2}\},$$

$$\phi_4=\{6s\ S_{1/2},\ 7s\ S_{-1/2},\ (6p)_0\ S_{1/2}\}.$$

The effect of this perturbation is to reduce f_{3776} to 0.059 as compared with the measured value 0.08.

This agreement between calculated and measured intensities indicates that Fermi and Segrè's explanation of the anomalous splitting ratio of $p_{1/2}$ and $p_{3/2}$ in terms of this perturbation must be essentially correct.

The nuclear magnetic moment is given by $g\mu_0 i$. Here μ_0 is the Bohr magneton, i the angular momentum of the nucleus in units of $h/2\pi$, and the g factor may be determined from the hyperfine structure splitting of a given level. The g factor found from Schüler and Keyston's[9] data on the $7s$ level of Tl I is compared with other determinations in Table I.

TABLE I.

	$s_{1/2}$	$p_{1/2}$	Most probable value according to Fermi
1840g	2.7	2.9	2.8

The $6p_{3/2}$ level is perturbed so strongly that one cannot rely on the g value determined from it. The g value for $p_{1/2}$ was calculated by Breit[4] and in this calculation the perturbation of $6s^26p$ by $6s6p7s$ was not taken into account. Calculation shows that this perturbation causes an increase in the g value of about 3 percent, but since the perturbed wave function for $p_{1/2}$ cannot be determined accurately, no significance can be attached to this correction.

In conclusion the writer wishes to thank Professor G. Breit for his helpful suggestions regarding this calculation, and for the use of tables of functions for the $6p$ states of Tl.

[9] Schüler and Keyston, Zeits. f. Physik **70**, 1 (1931).