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POSSIBLE EFFECTS OF NUCLEAR SPIN ON X-RAY TERMS

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Abstract

It is shown that magnetic moments of nuclei are likely to cause small but presumably measurable separations of x-ray terms. A nucleus having a spin of 9/2 (in units of $h/2\pi$) and a magnetic moment 9/2 in protonic units should cause the K terms of the heaviest elements to split into two components separated by about 22 volts. Such separations require for their detection a resolving power of 4200. For lighter elements the effect is relatively smaller. The same nuclear spin and magnetic moment would cause a separation of only 0.9 volts in Mo which would require for its detection a resolving power of 1.9×10^4

The calculations are made using Dirac's equation for a single electron without approximations. The effect of electrons in another shell, however, is neglected. It is estimated to be very small for a single K electron. If the observation of hyperfine structures in the K series of the heavier elements proves feasible, it should offer a simple means of determining magnetic moments of nuclei having a known spin.

THE hyperfine structure of spectral lines is at present attributed to the nuclear spin. The quantitative theory of the effect has been worked out by Hargreaves, Fermi, Goudsmit and Bacher and by Casimir.[1] A quantitative application of the theory is simple in a few cases such as e.g. the Li^+ hyperfine structure. For most spectra it is necessary to use approximate solutions for the electronic eigenfunctions which are at present usually carried out by the Hartree method. Quantitative determinations of the nuclear magnetic moment become, therefore, difficult. An examination of Fermi's result shows however that the order of magnitude of the effect can be expected to be much larger for the spectral terms in the x-ray region than for visible spectra. The absolute value of the splitting of an s term due to a single electron is according to Fermi

$$(F) \qquad (8\pi/3)[(2k+1)/k]\mu\mu_0\psi^2(0)$$

where k is the angular momentum of the nucleus, μ its magnetic moment, μ_0 the Bohr Magneton, and $\psi(0)$ is the value of the Schroedinger function

[1] J. Hargreaves, Proc. Roy. Soc. **A124**, 568 (1929). E. Fermi, Zeits. f. Physik **60**, 320 (1930). S. Goudsmit and R. F. Bacher, Phys. Rev. **34**, 1501, (1929). S. Goudsmit and L. A. Young, Nature, March 22, (1930).

at $r=0$. For large atomic numbers the value of $\psi(0)$ for a $(1s)K$ electron is large. In fact it is seen that $\psi^2(0)$ must increase as the cube of the reciprocal of the radius of the K orbit i.e., as Z^3 where Z is the atomic number. The energy of the K level increases only as Z^2 so that the splitting $\Delta\nu$ increases more rapidly than the term value ν. The values of the magnetic moments of the nuclei are not known at present and so it is necessary to be content with approximate estimates using the known orders of magnitude derived from hyperfine structure observations in the visible region. Making such estimates it is found that for heavy elements the separation $\Delta\nu$ may be expected to be of the order of 1/5000 of the frequency of the K line. The double crystal spectrometer developed by Bergen Davis appears to offer at least a possibility of observing such separations. The main purpose of this note is to call attention to the possibility of determining the magnetic moments of the nuclei by means of observations of the hyperfine structure of the lines in the K series. Corresponding effects in the L and M series are estimated to be smaller, though not necessarily beyond the range of experimental accuracy.

In order to form proper estimates for the case of x-rays it is necessary to perform somewhat more precise calculations than those of Fermi. The inaccuracy of his method lies in the fact that $E+(Ze^2/r)+mc^2$ is replaced by $2mc^2$. This is a good approximation as long as the region of large values of Ze^2/r is relatively small and as long as $E\sim mc^2$. Both of these conditions are satisfied for the lighter elements. The approximate dimensions of the regions in which the eigenfunction is appreciable are then of the order of 10^{-8} cm while $e^2/r>mc^2$ only if $r<2.5\times 10^{-13}$ cm. For the heavier elements this is not so because the charge density is more concentrated and Ze^2/r is greater for the same r. It thus becomes necessary to use exact solutions of Dirac's equation as a starting point in the calculation of the perturbation due to the magnetic moment of the nucleus.

Using Gordon's form of the solution of the Dirac equation for a Coulomb field of force[2] it is seen that for s terms of a single electron any set of four ψ's can be expressed as a linear combination of the following two sets

$$(I)\qquad \begin{aligned}\Psi_1 &= ((i/r)\cos\theta\phi_1, (i/r)\sin\theta e^{i\varphi}\phi_1, \phi_2/r, 0)\\ \Psi_2 &= ((i/r)\sin\theta e^{-i\varphi}\phi_1, -(i/r)\cos\theta\,\phi_1, 0, \phi_2/r)\end{aligned}$$

where ϕ_1, ϕ_2 are two functions (denoted by Gordon as ψ_1, ψ_2) given by

$$(G)\qquad \phi_1 = (1-E/mc^2)^{1/2}(\sigma_1-\sigma_2);\ \phi_2 = (1+E/mc^2)^{1/2}(\sigma_1+\sigma_2)$$

where $\sigma_1 = c_0^{(1)}e^{-k_0r}r^\rho F(-n'+1, 2\rho+1; 2k_0r);\ \ \rho = (1-\alpha^2)^{1/2}$

$$\sigma_2 = c_0^{(2)}e^{-k_0r}r^\rho F(-n', 2\rho+1; 2k_0r);\qquad \alpha = 2\pi Ze^2/hc$$

$$F(\alpha,\beta;x) = 1+\frac{\alpha x}{1!\beta}+\frac{\alpha(\alpha+1)x^2}{2!\beta(\beta+1)}+\cdots;\ k_0 = (2\pi mc/h)[1-(E/mc^2)^2]^{1/2}$$

$$c_0^{(1)}/c_0^{(2)} = -n'/[1+\alpha(1-(E/mc^2)^2)^{-1/2}];\ E/mc^2 = [1+\alpha^2/(n'+\rho)^2]^{-1/2}$$

Here $n'=0, 1, 2, \cdots$ for $(1s)$, $(2s)$, $\cdots$ terms.

[2] W. Gordon, Zeits. f. Physik **48,** 22 (1928).

In particular for $(1s)$ terms $c_0^{(1)}/c_0^{(2)}=0$ and σ_2 contains only one term.

The perturbation function due to the magnetic moment of the nucleus we take to be the same as Fermi's

$$w = (e/r^3)\vec{\alpha}[\vec{\mu} \times \vec{r}].$$

The unperturbed orthogonal Eigenfunctions can be taken to be

$$\begin{array}{l} u_k^{(1)}, u_{k-1}, \cdots, u_{-k}^{(1)} \\ \qquad u_k^{(2)}, \cdots, u_{-k+1}^{(2)}, u_{-k}^{(2)} \end{array} \tag{1}$$

corresponding to angular momenta

$$(k+\tfrac{1}{2}, k-\tfrac{1}{2}, \cdots, -k-\tfrac{1}{2})(h/2\pi)$$

To every angular momentum in the direction of the Z axis there correspond in general two unperturbed functions. Each of these is a rectangular matrix. The superscripts (1), (2) indicate wherther Ψ_1 or Ψ_2 of I are used. Thus the function $u^{(1)}{}_{k-l}$ has for elements zeros in the first l rows; Ψ_1 stands with its four elements in the lth row, and the remaining elements are zero. This is exactly as in Fermi's article. We remark that in the secular determinant we can have matrix elements only between such functions which are in the same vertical column of (1).

There are two multiple roots of the secular determinant one of which occurs $2k+2$ and the other $2k$ times. The functions at the extreme right and left correspond to the first of these two roots. This can be calculated first and the remaining root can be ascertained by obtaining the diagonal elements of the subdeterminant formed by the combinations of any other vertical pair in (1). The first root is therefore $\int u_k^{*(1)} w\, u_k^{(1)}\, d\tau$. This integral sign is of course understood to include in it a summation over the indices of the matrix eigenfunctions. The operations μ are on the columns and the operations α are on the rows. We are therefore only interested in that part of $wu_k^{(1)}$ which on performing the operations μ involves the index k. This part is due to μ_z and is $(e\mu/r^3)\,(x\alpha_y - y\alpha_x)u_k^{(1)}$. The remaining operation is entirely on Ψ_1. Performing it and substituting in the intergral it is found that

$$w_1 = \int u_k^{(1)*} w u_k^{(1)} d\tau = (16\pi/3)e\mu \int_0^\infty (\phi_1\phi_2/r^2)dr \tag{2}$$

This is therefore one of the roots. The sum of the two roots is $\int[u_{k-1}^{(1)*}\, w\, u_{k-1}^{(1)} + u_k^{(2)*}\, w\, u_k^{(2)}]\, d\tau$, with the same understanding about the integral as before. The calculation of the first term in brackets is the same as before with the difference that a factor $(k-1)/k$ is introduced. In the second term the result (2) is obviously obtained but with opposite sign due to the occurrence of Ψ_2 instead of Ψ_1. The sum of the two roots is therefore

$$w_1 + w_2 = -\, w_1/k. \tag{3}$$

Hence

$$\Delta\nu = w_1 - w_2 = ((2k+1)/k)w_1. \tag{4}$$

The difference between this result and Fermi's can be expressed by saying that Fermi's

$$\psi^2(0) \rightarrow (2e/\mu_0)\int_0^\infty (\phi_1\phi_2/r^2)dr = -(8\pi mc/h)\int_0^\infty (\phi_1\phi_2/r^2)dr.$$

Equation (4) is practically exact for any s term; in a Coulomb field the only approximation made being that of supposing the effect of the nuclear magnetic moment to be small.

In applying (4) it must be remembered that ϕ_1, ϕ_2 are supposed to be normalized in such a way that

$$4\pi\int(\phi_1^2+\phi_2^2)dr = 1 \tag{5}$$

as is obvious from (I). For (1s) terms

$$\phi_1 = -C[1-(E/mc^2)]^{1/2}e^{-k_0 r}r^\rho;\ \phi_2 = C[1+(E/mc^2)]^{1/2}e^{-k_0 r}r^\rho. \tag{6}$$

These expressions are substituted into (4), the normalization constant C being determined by (5). The integrals are expressible by means of the Γ function. Using $\Gamma(x+1)=x\Gamma(x)$ and the relations G it is found that the exact quantity which replaces Fermi's $\psi^2(0)$ is (see (4′))

$$(4\pi mc/h)^3(\alpha^3/8\pi)[2\rho^2-\rho]^{-1}. \tag{7}$$

Here the first two factors are Fermi's $\psi^2(0)$. and the factor in brackets is a correction due to relativity effects brought in by this calculation.* Substituting (7) into (F)

$$\begin{aligned}\Delta\nu &= 0.0169Z^3(k+\tfrac{1}{2})(1840\mu/2k\mu_0)[2\rho^2-\rho]^{-1}\,\text{cm}^{-1}\\ &= 2.08(Z/100)^3(k+\tfrac{1}{2})(1840\mu/2k\mu_0)[2\rho^2-\rho]^{-1}\,\text{volts}.\end{aligned} \tag{8}$$

In order to estimate the order of magnitude of the effect we suppose that $k=9/2$ and that $1840\mu=2k\mu_0$. We find for

	U	Bi	W	Mo
Z =	92	83	74	42
$\Delta\nu$ =	22.5	12.6	7.31	0.896 volts
$\nu_{K\alpha}$ =	(9.395	7.436	5.912	1.734)$\times 10^4$ volts
$\nu_{K\alpha}/\Delta\nu$ =	4175	5911	8092	19361

Of these elements Bi is known[3] to have a nuclear spin 9/2. It is clear from the above table that for the heavier elements the separation is sufficiently large not to be confused with chemical effects and that the resolving power tabulated in the last row is sufficiently small to make the possibility of experimental detection of $\Delta\nu$ at least hopeful.

In a similar way the separation of 2s terms has been worked out. In this case the correction factor to Fermi's formula is

$$[2/(1+\rho)]^{3/2}[1+(2\rho+2)^{1/2}]\cdot[\rho(4\rho^2-1)]^{-1}.$$

* In fact it is readily found that $\psi^2(0)=1/\pi a_0^3n^3$ where $a_0=h^2/(4\pi^2mZe^2)$ and n is the total quantum number.

[3] E. Back and S. Goudsmit, Zeits. f. Physik **43**, 321 (1927); **47**, 174 (1928).

This correction factor is even larger than that derived for $1s$ electrons. For U it is 3.94. Neglecting screening the splitting of the L_{11} level of U can be expected to be $3.94/2.78\times(1/8)=1/5.64$ of the K level splitting. For the lighter elements this fraction approaches 1/8. It is presumably much less accurate however to apply the present method of calculation to the L electrons because screening effects must be more important here. Their importance may be expected to be least for the heaviest elements. The order of magnitude of the splitting of the L_{11} level of U supposing its nucleus to have a spin 9/2 and a magnetic moment 9/2 proton units is 4.0 volts. The frequency of the L_{11}—M_{21} line of the L series is 1221×13.55 volts. For the L series $\nu/\Delta\nu$ is therefore also of the order 4150. This estimate is, however, not as accurate as the one for the K series on account of the screening effects. It is mentioned here only because it is of interest to see that the same order of magnitude of the splitting can be expected for both series and because the L series is more accessible experimentally.[4]

The writer is very grateful to Dr. E. Wigner for an interesting discussion.

[4] A single observation of the fine structure separation of the K levels gives only $(2k+1)\mu/k$. In order to obtain μ it will be necessary to determine k either by optical means (band spectra, hyperfine structure) or else by observing multiplicities of other X terms, or perhaps by intensity measurements of the hyperfine structure components in the K series.