DERIVATION OF HYPERFINE STRUCTURE FORMULAS FOR ONE ELECTRON SPECTRA

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(Received November 24, 1930)

Abstract

A short but rigorous derivation is given for the energy level separations caused by a nuclear magnetic moment in a one electron spectrum. Formulas (5) and (7) are general. For weak coupling between the orbital angular momentum and the electron spin formula (6) may be used.

FORMULAS for the hyperfine structure of one electron spectra have been derived by numerous authors.[1] The calculations are in most cases very lengthy and are carried out for special cases. The results may be obtained by the following short and yet rigorous consideration. The interaction energy of a nucleus with an electron of charge $-e$ may be represented by

$$H' = g\mu_0(\mathbf{A}\cdot\mathfrak{y}) \tag{1}$$

where $\mathfrak{y}$ is the angular momentum matrix vector of the nucleus in units $h/2\pi$ and $g\mu_0\mathfrak{y}$ is its magnetic moment. μ_0 is the Bohr magneton and g is a numerical factor to be determined by comparison with experiment. Here

$$\mathbf{A} = 2\mu_0[r^{-3}\mathbf{L} - \mathfrak{d}r^{-3} + 3\mathbf{r}(\mathbf{r}\mathfrak{d})r^{-5}]/[1 + (eA_0/2mc^2)] + 2\mu_0[\mathfrak{d}r^{-2} - \mathbf{r}(\mathbf{r}\mathfrak{d})r^{-4}]\frac{d}{dr}[1 + (eA_0/2mc^2)]^{-1} \tag{2}$$

$\mathbf{L}$ is the orbital angular momentum in units $h/2\pi$, $2\mathfrak{d}$ is Pauli's spin vector so that $(h/2\pi)\mathfrak{d}$ is the angular momentum of the electron spin, r is the distance from the nucleus and A_0 is the electrostatic potential. Expression (2) may be derived from the Dirac equation by eliminating two wave functions. The first part of (2) is the only important one except for s terms where the second part is responsible for all of the effect. The total angular momentum is

$$\mathbf{F} = \mathbf{J} + \mathfrak{y} = \mathbf{L} + \mathfrak{d} + \mathfrak{y}. \tag{3}$$

The quantum number of $\mathbf{F}$, $\mathbf{J}$, $\mathbf{L}$, $\mathfrak{y}$ we write as f, j, l, i. By well-known theorems about angular momenta we have for the perturbed energy

$$w = g\mu_0(\mathbf{AJ})_j[f(f+1) - i(i+1) - j(j+1)]/[2j(j+1)]. \tag{4}$$

Here $(\mathbf{AJ})_j$ is the value of any diagonal element in the matrix $(\mathbf{AJ})$ in that part of it which belongs to the quantum number j. Substituting $\mathbf{J}=\mathbf{L}+\mathfrak{d}$ into $(\mathbf{AJ})$ we have except for s terms

[1] J. Hargreaves, Proc. Roy. Soc. **124**, 568 (1929); **127**, 141, 407 (1930). E. Fermi, Zeits.f. Physik **60**, 320 (1930). Unpublished calculations of Casimir quoted in Pauling and Goudsmit's book.

$$(\boldsymbol{AJ})/2\mu_0 = -\boldsymbol{\delta}^2 r^{-3} + 3(\boldsymbol{r}\boldsymbol{\delta})^2 r^{-5} + 3(\boldsymbol{rL})(\boldsymbol{r}\boldsymbol{\delta})r^{-5} + r^{-3}\boldsymbol{L}^2.$$

The denominator of the first part of (2) being set here $=1$ since $eA_0/2mc^2$ is in this case small. We note that $\boldsymbol{rL}=0$ and that $3(\boldsymbol{r}\boldsymbol{\delta})^2 - r^2\boldsymbol{\delta}^2 = 0$. We have then

$$w = g\mu_0{}^2(r^{-3}\boldsymbol{L}^2)_j[f(f+1) - i(i+1) - j(j+1)]/[j(j+1)]. \tag{5}$$

This is exact since the coupling to the nucleus is weak. If in addition the coupling of $\boldsymbol{L}$ and $\boldsymbol{\delta}$ is weak we may write $\boldsymbol{L}^2 = l(l+1)$ so that

$$w = g\mu_0{}^2\frac{l(l+1)}{j(j+1)}[f(f+1) - i(i+1) - j(j+1)]\overline{(r^{-3})} \tag{6}$$

For s terms the denominator $1+(eA_0/2mc^2)$ insures the disappearance of the first part of (2) in the approximation of formula (5). In this case

$$(\boldsymbol{AJ})_j = 2\mu_0\int_0^\infty \psi^2(r)(1/2r^2)\left\{\frac{d}{dr}[1 + (eA_0/2mc^2)]^{-1}\right\}4\pi r^2 dr \doteqdot 4\pi\mu_0\psi^2(0) \tag{6'}$$

in the same approximation as Fermi's.[2] If therefore we add to (6) the statement that for $l=0$

$$[\overline{(r^{-3})}l(l+1)]_{l=0} = 2\pi\psi^2(0) \tag{7}$$

formula (6) becomes complete.

These results in the approximation of equation (6) are in complete agreement with the statements made in Pauling and Goudsmit's book where the calculations of Casimir have been used.

[2] The exact formula for a Coulomb field is found in G. Breit Phys. Rev. **35, 1447 (1930).**