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Analytic determination of the hyperfine-assisted Zeeman shift for the deuterium atom

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Small extra Zeeman shifts measured in the ground states of ^{85}Rb and ^{87}Rb have previously been shown to be due to the hyperfine interaction to second order coupled with the Zeeman interaction to first order. Approximate theoretical calculations yielded effective frequencies for the two isotopes of 0.016 Hz/T and 0.18 Hz/T, respectively, in good agreement with experiments. We calculate exactly the same shift for the 1s and 2s states of ^{2}H by perturbation differential equations. For the 1s and 2s states the respective frequencies are 2.61×10^{-5} Hz/T and 2.56×10^{-5} Hz/T.

Recently, Fletcher, Lipson, and Larson[1] through high precision measurements of the hyperfine and Zeeman interactions in ^2S ground-state Rb atoms found evidence for an additional term in the ground energy of the form

$$E(M_I,M_s)=\frac{h\beta M_I^2 M_s B}{1/2}\ , \tag{1}$$

where M_I and M_s are, respectively, the nuclear and electron spin magnetic quantum numbers. The measured value of β for ^{87}Rb was

$$\beta=0.168(15)\ \text{Hz/T}\ . \tag{2}$$

Fortson[2] has shown that this energy is due to a third-order perturbation-theory term which is second order in the contact hyperfine interaction and first order in the Zeeman interaction. Using the standard sum-over-states expression for the term, along with approximations to the energy differences, he obtained

$$\beta=0.18\ \text{Hz/T}\ , \tag{3}$$

in good agreement with the ^{87}Rb experiment. The ^{85}Rb result was shown to be simply related to the ^{87}Rb value because they scale as g_I^2, where g_I is the nuclear g factor.

Interestingly, this effect has never been seen or calculated for the ^{2}H atom. Although the calculation for ^{1}H is identical to that which follows, the effect is trivial: the $\pm\frac{1}{2}$ nuclear spin lines are shifted equally. In this note we calculate this interaction exactly for ^{2}H. Besides its intrinsic merit, the ^{2}H-atom result will be useful in future testing of approximate methods.

The fundamental Hamiltonian which we consider is

$$H=H^0+H^B+H^C\ , \tag{4}$$

where

$$H^0=-\tfrac{1}{2}\nabla^2-\frac{1}{r}\ . \tag{5a}$$

$$H^C=\frac{8\pi}{3}\mu_B^2 m_p^{-1} g_e g_D \delta^3(\mathbf{r})\mathbf{I}\cdot\mathbf{S}\ , \tag{5b}$$

and

$$H^B=\mu_B g_e \mathbf{B}\cdot\mathbf{S}\ . \tag{5c}$$

Atomic units are used, and $g_D=0.857$. Following Fortson,[2] we, too, neglect the nuclear Zeeman term and tensor hyperfine coupling.

Although the perturbation theory is of third order, we shall show that all that is needed is the wave function which is first order in H^C. We may obtain this wave function directly,[3] circumventing the usual sum over states. Since we are only concerned with s states we may write the zeroth-order wave function as

$$\psi^0_{n_s m_s m_I}(\mathbf{r})=\varphi_{n_s}(\mathbf{r})\,|\,m_I m_s\rangle\ , \tag{6}$$

where we have used the high field eigenstates of H as a basis in spin space, and $\varphi_{n_s}(\mathbf{r})$ are s orbitals.

In principle there will be two first-order wave functions, $\psi^B_{n_s m_s m_I}$ and $\psi^C_{n_s m_s m_I}$. Since H^B commutes with H^0, however, $\psi^B_{n_s m_s m_I}$ is zero. The derived energy term being second order in H^C and first order in H^B is readily shown to be

$$E_{n_s}(m_s m_I)=\int d^3\mathbf{r}(\psi^C_{n_s m_s m_I})^*(H^B-E^B_{m_s})\psi^c_{n_s m_s m_I}\ , \tag{7}$$

where $E^B_{m_s}$ is the first-order Zeeman energy

$$E^B_{m_s}=\mu_B g_e m_s B\ . \tag{8}$$

Since the zeroth-order energy is $2(2I+1)$-fold degenerate, care must be taken in solving for $\psi^C_{n_s m_s m_I}$. Failure to do so results in unsolvable differential equations and singular sums over states.[2] Writing down the first-order perturbation equation in the coupled F,m_F representation, in which H^C is diagonal, and transforming to the high-field representation shows that

$$\psi^C_{n_s m_s m_I}=\tfrac{2}{3}\mu_B^2 m_p^{-1} g_e g_D \varphi^c_{n_s}(r)\mathbf{I}\cdot\mathbf{S}\,|\,m_I m_s\rangle\ , \tag{9}$$

where $\varphi^c_{n_s}$ is determined by the inhomogeneous equation

$$(H^0-E^0_{n_s})\varphi^c_{n_s}+4\pi[\delta(\mathbf{r})-\phi^2_{n_s}(0)]\varphi_{n_s}=0\ . \tag{10}$$

The energy becomes

$$E_{n_s}(m_s,m_I) = \tfrac{4}{9}\mu_B^5 m_p^{-2} g_e^3 g_D^2 [\langle m_s m_I \,|\, (\mathbf{I}\cdot\mathbf{S})(\mathbf{B}\cdot\mathbf{S})(\mathbf{I}\cdot\mathbf{S}) \,|\, m_s m_i \rangle - m_s B \langle m_s m_I \,|\, (\mathbf{I}\cdot\mathbf{S})^2 \,|\, m_s m_I \rangle] \times \int (\varphi_{n_s}^c)^2 d\mathbf{r} \,. \tag{11}$$

Reduction of the spin matrix elements[2] yields

$$E_{n_s}(m_s m_I) = \tfrac{2}{9}\mu_B^5 B m_p^{-2} g_e^3 g_D^2 [m_s m_I^2 - (I+1)m_s + \tfrac{1}{2}m_I] \times \int (\varphi_{n_s}^c)^2 d\mathbf{r} \,. \tag{12}$$

Equation (10) has been solved by Schwartz[3] for $n=1$ and 2. The solutions have been used for other purposes.[3,4] Requiring $\varphi_{n_s}^c$ to be orthogonal to φ_{ns}, and using $\gamma = 1.7811\ldots$ (a form of Euler's constant[5]), the wave function may be written as

$$\varphi_{1s}^c = \left[\frac{2}{r} + 4\ln(2\gamma r) - 10 + 4r\right] \frac{e^{-r}}{\sqrt{\pi}} \tag{13a}$$

and

$$\varphi_{2s}^c = \left[\frac{4}{r} - 8\ln(\gamma r) + 6 + 4r\ln(\gamma r) - 13r + r^2\right] \frac{e^{-r/2}}{\sqrt{32\pi}} \,. \tag{13b}$$

The integrals may be evaluated, giving

$$\int (\varphi_{1s}^c)^2 d\mathbf{r} = \frac{8\pi^2}{3} + 28 \,, \tag{14a}$$

and

$$\int (\varphi_{2s}^c)^2 d\mathbf{r} = \frac{8\pi^2}{3} + 27 \,, \tag{14b}$$

which are surprisingly close in value. β_{1s} and β_{2s} for ^{2}H may now be obtained realizing that

$$\frac{\mu_B g_e}{h} = 2.8\times 10^{10} \text{ Hz/T} \,.$$

The results are

$$\beta_{1s} = 2.61\times 10^{-5} \text{ Hz/T} \tag{15}$$

and

$$\beta_{2s} = 2.56\times 10^{-5} \text{ Hz/T} \,. \tag{16}$$

The results are far smaller than those obtained for Rb since Z is much smaller in H.

The approach described above may readily be generalized to any state of any hydrogen isotope or hydrogenlike ion. For alkali-metal atoms the analogous technique involving a numerical or basis-function solution of the radial differential equation is likely to be an efficient method.

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