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Nuclear Magnetic Moments and Atomic Hyperfine Structure

AAGE BOHR*
Department of Physics, Columbia University, New York, New York
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The asymmetric nuclear model discussed in a previous paper provides the basis for a more detailed interpretation of nuclear magnetic moments than the single particle model permits. The structure of the moment which the model implies may be tested by a study of the influence of the finite size of the nucleus on the atomic h.f.s. This effect was investigated previously in cooperation with Weisskopf, and is considered more closely in the present paper with the assumption that the nuclei in question can be described in terms of a single particle moving in an asymmetric nuclear core. The K-isotopes should be well represented by this model, and for these nuclei the theoretical value obtained for the h.f.s. is in close agreement with the observed data. Also for the Rb-isotopes the agreement is satisfactory.

I. INTRODUCTION

IN a recent article[1] a nuclear model was discussed in which the individual nucleons are assumed to move in an average nuclear field which deviates from spherical symmetry. This so-called asymmetric model contains many of the characteristic features of the single particle model, and at the same time incorporates such collective types of nuclear motion as are manifested in the existence of the large electric quadrupole moments.

The asymmetric model implies that the nuclear core possesses rotational degrees of freedom. The character of a nuclear state, and its magnetic moment in particular, is therefore not determined uniquely by the quantum numbers of the single particle motion, but depends also on the coupling of this motion to the asymmetric nuclear core and on the rotational state of the nucleus. For a given total angular momentum of the nucleus the magnetic moment may have any value, within certain limits, corresponding to the observed behavior of nuclear magnetic moments.

In the present state of our knowledge of the coupling of angular momenta in the nucleus, it is in general difficult to make quantitative predictions regarding the value of the magnetic moment. By means of the empirical value of the moment it is possible, however, to determine the character of the nuclear state in question, at any rate for the simplest type of nuclei, those which can be described in terms of a single nucleon moving in a nuclear core which possesses no intrinsic angular momentum.

A detailed model of the nucleus is thereby obtained which can be tested in its relation to other nuclear properties. One such test is provided by an accurate measurement of the atomic hyperfine structure. Because of the distribution of the magnetic moment over the finite volume of the nucleus, the h.f.s. splitting differs slightly from the value corresponding to a point-dipole at the nuclear center. This deviation, the h.f.s. anomaly, depends not only on the size of the nucleus, but also on the intrinsic structure of the moment. Effects of this type have been observed in a number of cases.[2–5]

A theoretical treatment of the h.f.s. anomaly for the case of heavy nuclei was given previously by Weisskopf and the writer.[6] It was found that the part of the nuclear moment due to the intrinsic spin of the nucleons, and the part due to orbital motion in the nucleus, will contribute differently to the h.f.s. anomaly. The effect is therefore especially sensitive to the distribution of the

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[1] A. Bohr, Phys. Rev. 80, 134 (1951). Referred to in the following as A. See also J. Rainwater, Phys. Rev. 79, 432 (1950).

[2] J. E. Nafe and E. B. Nelson, Phys. Rev. 73, 718 (1948).

[3] F. Bitter, Phys. Rev. 76, 150 (1949).

[4] P. Kusch and A. K. Mann, Phys. Rev. 76, 707 (1949).

[5] Ochs, Logan, and Kusch, Phys. Rev. 78, 184 (1950).

[6] A. Bohr and V. Weisskopf, Phys. Rev. 77, 94 (1950). Referred to in the following as B.

nuclear moment on these two types of magnetic moment.

Since no model was then available which could account in detail for the nuclear moments, an approximate estimate of the h.f.s. anomaly was made on the basis of very general assumptions regarding the structure of the nucleus. In the following, we shall attempt a more accurate treatment based on the asymmetric nuclear model. For simplicity, we shall assume that the nuclei in question can be represented in terms of a single nucleon moving with respect to the nuclear core.

II. ANGULAR DISTRIBUTION OF THE SPIN MOMENT

In order to evaluate the h.f.s. anomaly for the spin part of the moment, the assumption was made in **B** that this part of the moment can be represented by a spherically symmetric distribution function. Such an assumption is justified for nuclear models, like the uniform model,[7] which ascribe no exceptional spatial distribution to the nucleons carrying the spin moment. The single particle model, or the asymmetric model, however, implies in general pronounced angular asymmetries in the spin distribution, which may have a considerable influence on the h.f.s. anomaly.

The effect of such asymmetries is given by formula (**B**7). It follows from [**B**(6, 8, and 12)] that the quantity κ_s—representing the anomaly in the spin part of the h.f.s.—must be replaced by κ_s' given by

$$\kappa_s' = \kappa_s + \zeta(\kappa_s - \kappa_L), \tag{1}$$

where

$$\zeta = \frac{-1}{(s_z)_{\text{Av}}}\Big((s_x\cos\varphi + s_y\sin\varphi)\tfrac{3}{2}\cos\vartheta\sin\vartheta + s_z(\tfrac{3}{2}\cos^2\vartheta - \tfrac{1}{2})\Big)_{\text{Av}}, \tag{2}$$

the averages to be taken for the spin and angular distribution of the odd nucleon in the nucleus.

Extreme Single Particle Model

We first consider the extreme single particle model according to which the total nuclear angular momentum is possessed by the odd nucleon.

The angular distribution and the spin direction of this nucleon are given by the wave functions

$$\psi_+ = Y_{I-\frac{1}{2}}^{I-\frac{1}{2}}(\vartheta, \varphi)\chi^+ \tag{3a}$$

and

$$\psi_- = \frac{1}{(2I+2)^{\frac{1}{2}}} Y_{I+\frac{1}{2}}^{I-\frac{1}{2}}(\vartheta, \varphi)\chi^+ - \left(\frac{2I+1}{2I+2}\right)^{\frac{1}{2}} Y_{I+\frac{1}{2}}^{I+\frac{1}{2}}(\vartheta, \varphi)\chi^- \tag{3b}$$

for the cases of parallel and antiparallel spin and orbital moment, respectively. The total angular momentum is denoted by I, and we are considering the magnetic substate $M=I$. The angular wave functions Y_l^m are the normalized spherical harmonics[8] representing a particle with angular momentum l and magnetic quantum number m. The spin functions χ^+ and χ^- correspond to the eigenvalues $s_z=\frac{1}{2}$ and $s_z=-\frac{1}{2}$, respectively.

The evaluation of ζ gives

$$\zeta = (2I-1)/4(I+1), \quad (I=l+\tfrac{1}{2}) \tag{4a}$$

and

$$\zeta = (2I+3)/4I, \quad (I=l-\tfrac{1}{2}) \tag{4b}$$

for the states (3a) and (3b), respectively.

The asymmetry expressed by the quantity ζ is partly due to the fact that, for $I>\frac{1}{2}$, the particle density is not isotropic, but is a maximum for $\vartheta=\pi/2$. Thus, it is evident from the expressions (2) that ζ approaches the value $\frac{1}{2}$ for large I.

In the case of antiparallel **l** and **s**, an additional effect arises from the fact that the direction of the spin depends on the polar angles of the particle. By means of the recursion formula

$$Y_{I+\frac{1}{2}}^{I-\frac{1}{2}} = -(2I+1)^{\frac{1}{2}}\cot\vartheta\cdot e^{-i\varphi}\cdot Y_{I+\frac{1}{2}}^{I+\frac{1}{2}} \tag{5}$$

the wave function (3b) may be written:

$$\psi_- = f(\vartheta, \varphi)\{\cos\vartheta e^{-\frac{1}{2}i\varphi}\chi^+ + \sin\vartheta e^{\frac{1}{2}i\varphi}\chi^-\}. \tag{6}$$

It follows that the direction of the spin is characterized by the polar angles 2ϑ and φ. It is easily seen that this effect tends to increase ζ by making the magnetic field inside the nucleus depart more strongly from the field produced by a dipole at the nuclear center.

Asymmetric Model. Extreme Coupling Cases

For the asymmetric model, the nuclear wave function is not determined uniquely by the values of I and M, even if we restrict ourselves to the ground state of the nucleus. As discussed in **A**, a number of different coupling cases may arise, depending on the strength of the spin-orbit coupling as compared with the coupling of the nucleon to an axis of the nucleus and the rotational level-spacing of the nucleus.

In the case B_2 (see **A**), of very strong spin-orbit coupling, the particle wave function is again given by (3), except for the fact that the polar angles of the particle are now defined with respect to the axis of the nucleus, and that the spin functions represent states for which the spin is quantized parallel or antiparallel to the nuclear axis. We assume that the asymmetry of the nuclear core is not too large, and that l therefore is a good quantum number. To obtain the wave functions for the entire nucleus, the expressions (3) must be multiplied by the symmetrical top wave function

[7] H. Margenau and E. Wigner, Phys. Rev. **58**, 103 (1940).

[8] The phase factors are those used in E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, 1935).

describing the motion of the nuclear axis, whose polar angles we denote by θ and ϕ.

It is easily seen from (2) that the value of ζ for a nuclear state of this type is equal to the value obtained from the single particle model. In fact, the numerator as well as the denominator of (2) represent the z-component of a vector. If we first keep θ and ϕ fixed, and average over the motion of the particle with respect to the nuclear axis, these two vectors must, for symmetry reasons, have the direction of the nuclear axis. Their ratio is equal to (4), and is not affected by the subsequent averaging with respect to θ and ϕ.

If the spin-orbit coupling is smaller than the coupling of **l** to the nuclear axis, but larger than the rotational level spacing of the nucleus, we have the coupling case B_1. The wave function describing the motion of the nucleon with respect to the nuclear axis is given by

$$\psi_+ = Y_{I-\frac{1}{2}}^{I-\frac{1}{2}}(\vartheta', \varphi')\chi^+ \quad (I=l+\tfrac{1}{2}) \tag{7a}$$

and

$$\psi_- = Y_{I+\frac{1}{2}}^{I+\frac{1}{2}}(\vartheta', \varphi')\chi^- \quad (I=l-\tfrac{1}{2}), \tag{7b}$$

where ϑ' and φ' are the polar angles of the particle in the nuclear coordinate system.

In case of parallel **l** and **s**, the coupling cases B_1 and B_2 are identical, but for antiparallel **l** and **s** the spin direction given by (7b) does not have the dependence on the polar angles which is characteristic of the wave function (3b). The value of ζ for the state (7b) is simply obtained from (4a) by replacing I with $I+1$. Thus

$$\zeta = (2I-1)/4(I+1), \quad (I=l+\tfrac{1}{2}) \tag{8a}$$

and

$$\zeta = (2I+1)/4(I+2), \quad (I=l-\tfrac{1}{2}) \tag{8b}$$

for the states (7a) and (7b), respectively. For small I, the expression (8b) gives values for ζ much smaller than those obtained from (4b).

Finally, if the spin-orbit coupling is smaller than the nuclear rotational level-spacing, we have the coupling case A. The nuclear wave function is given by an expression of the type (3) except that the spherical harmonics must be replaced by wave functions which describe the rotation of the nuclear core as well as the orbital motion of the particle with respect to the nuclear axis.

We first consider the parallel case corresponding to (3a). From (2) it follows that ζ is given by

$$\zeta = -(\tfrac{3}{2}\cos^2\vartheta - \tfrac{1}{2})_{\text{Av}}, \tag{9}$$

where ϑ is the polar angle of the nucleon with respect to the fixed z-axis. In order to evaluate (9) it is convenient to express ϑ in terms of the polar angle ϑ' with respect to the nuclear axis. One finds

$$\zeta = -(\tfrac{3}{2}\cos^2\vartheta' - \tfrac{1}{2})_{\text{Av}}(\tfrac{3}{2}\cos^2\theta - \tfrac{1}{2})_{\text{Av}}, \tag{10}$$

which leads to

$$\zeta = (I-1)(2I-1)^2/4(2I+1)(I+1)^2 \tag{11a}$$

for the state in question.

For antiparallel **l** and **s**, corresponding to (3b), the coupling cases A and B_1 are identical. The value of ζ is therefore given by (8b).

Asymmetric Model. Intermediate Coupling Cases

The empirical nuclear magnetic moments do not, in general, coincide with either of the values corresponding to the three extreme coupling cases considered above. As was pointed out in **A**, it is possible, however, at any rate for the simplest types of nuclei, to account for the magnetic moments in terms of intermediate coupling cases. For the following applications we shall consider coupling cases between B_1 and B_2.

The case of $l=I-\frac{1}{2}$, in which the two models B_1 and B_2 coincide, needs no further treatment. For $l=I+\frac{1}{2}$, the wave function describing the motion of the particle with respect to the nuclear axis will be of the general form:

$$\psi_- = \text{const.}(Y_{I+\frac{1}{2}}^{I-\frac{1}{2}}\chi^+ + \beta Y_{I+\frac{1}{2}}^{I+\frac{1}{2}}\chi^-). \tag{12}$$

The value of β depends on the strength of the $l-s$ coupling compared with the coupling of **l** to the nuclear axis.

An evaluation of (2) leads to

$$\zeta = \frac{1}{4(I+2)}\frac{1}{\beta^2-1}\{\beta^2(2I+1) - 6\beta(2I+1)^{\frac{1}{2}} + 5 - 2I\}. \tag{13}$$

It will be noted that, for $\beta = -(2I+1)^{\frac{1}{2}}$ and $\beta = \infty$, expression (13) coincides with (4b) and (8b), respectively.

III. THE ORBITAL ANGULAR MOMENTUM

The expression given in **B** for κ_L—representing the anomaly in the orbital part of the h.f.s.—has a simple interpretation if the orbital angular momentum can be ascribed to a single particle. It is therefore immediately applicable to the extreme single particle model.

According to the asymmetric model, the nuclear core also contributes to **L**. For the corresponding part of the nuclear magnetic moment, the value of κ can be obtained from an expression like (**B**12) if only the radial average is performed for the radial distribution of the orbital magnetic moment in the nuclear core.

Since the contribution of the nuclear rotation to the magnetic moment of the nucleus is in general small, one obtains a first approximation by neglecting the difference between the distribution of the orbital magnetic moment in the core and the radial density distribution of the single particle. The expression (**B**12) can then be used for the total orbital magnetic moment of the nucleus. It must be taken into account, however, that, due to the contribution of the nuclear core, the effective orbital g-factor, g_L, differs somewhat from the single particle value.

IV. RADIAL AVERAGES

According to (**B**18), the radial averages of κ_s and κ_L involve essentially the mean value of $(R/R_0)^2$ for the density distribution of the odd particle. The nuclear radius is denoted by R_0.

On the average, for all the particles in the nucleus, this mean value equals $\frac{3}{5}$, if the nuclear density is constant. For the individual nucleons, however, $(R/R_0)^2_{\text{Av}}$ will depend on the kinetic energy and angular momentum and may differ appreciably from $\frac{3}{5}$.

As an indication of the trend of $(R/R_0)^2_{\text{Av}}$, it may be noted that in the semiclassical approximation, valid for large quantum numbers, one obtains, for a particle confined within a sphere of constant potential,

$$(R/R_0)^2_{\text{Av}}=\tfrac{1}{3}+\tfrac{2}{3}(l^2\hbar^2/2MTR_0^2) \qquad (14)$$

where T is the kinetic energy of the particle, M its mass.

In individual cases, an estimate of $(R/R_0)^2_{\text{Av}}$ can be made by assuming the orbit to have the quantum numbers given by the single particle model on the basis of the nuclear spin and the empirical value of the magnetic moment. If the potential is assumed to vanish for $R>R_0$, and for $R<R_0$ to be a constant, which can be determined from the empirical value of the binding energy, the entire particle wave function can then be constructed.

If the odd nucleon is a proton, the influence of the Coulomb forces should be taken into account. This effect is in general rather small, and, since the electrostatic potential does not vary greatly over the region in which the particle spends most of its time, the potential can be approximated by a constant equal to the Coulomb potential at the nuclear surface. This amounts to the introduction of an effective binding energy given by the energy which the proton must acquire in order to be able to leave the nucleus by passing over the barrier.

V. FORMULAS FOR THE H.F.S. ANOMALY

From (1) and (**B**18), one gets the following expression:

$$\epsilon=-\{(1+0.38\zeta)\alpha_s+0.62\alpha_L\}(R/R_0)^2 \qquad (15)$$

for the h.f.s. anomaly as a fraction of the h.f.s. for a point nucleus. The quantity b is a function of Z and R_0 and is tabulated in **B**.

The fractions of the nuclear moment of spin type and orbital type are denoted by α_s and α_L, respectively. These quantities are given by (**B**20) in terms of the nuclear g-factors. For the asymmetric model, however, the orbital g-factor depends on the contribution of the nuclear core to the magnetic moment of the nucleus and must itself be determined from the empirical value of the nuclear moment.

We shall in particular consider nuclei for which the angular momentum coupling falls between that of the cases B_1 and B_2. The contribution of nuclear rotation to the magnetic moment is then given by (**A**1). In the extreme cases, B_1 and B_2, the value of g_Ω is given by (**A**2) and (**A**3) respectively, but more generally we have

$$Ig_\Omega=\sigma g_s+(I-\sigma)g_l, \qquad (16)$$

where σ represents the average value of the odd particle spin component along the nuclear axis. This quantity is given by

$$\sigma=(1-\beta^2)/2(1+\beta^2) \qquad (17)$$

in terms of the coefficient β in the wave function (12)

From (16) and (**A**1) one obtains

$$\sigma=[(I+1)g_I-g_R-Ig_l]/(g_s-g_l), \qquad (18)$$

where g_R is the g-factor for the nuclear rotation. Its value is somewhat uncertain, but is expected to be of the order of Z/A.

Expression (18) gives σ in terms of the empirical value of g_I. The quantities α_s and α_L are then determined by

$$\alpha_s=\sigma g_s/(I+1)g_I, \quad \alpha_L=1-\alpha_s. \qquad (19)$$

Moreover, (17) gives the value of β from which ζ can be found by means of (13).

It should be noted that (17) gives only the numerical value of β, while ζ depends also on the sign of β. For a particle moving in a field of cylindrical symmetry, there are two eigenstates of the type (12), one with positive and one with negative β. It is easily seen that if the spin orbit coupling favors large j (parallel coupling of **l** and **s**), the state of positive β has the lowest energy. If the sign of the spin orbit coupling is reversed, β must be taken to be negative for the state of lowest energy.

VI. DISCUSSION OF EXPERIMENTAL DATA

K

A particularly instructive example of h.f.s. anomalies is provided by the recent accurate measurement by Ochs, Logan, and Kusch[5] of the nuclear moments of the odd K-isotopes and of the h.f.s. of the ground states of the corresponding atoms. In fact, the K-nuclei ($Z=19$) contain just one proton less than the number required for a closed shell. These nuclei are expected to be well represented by the model of a single particle moving in a nuclear core of no intrinsic angular momentum. Their magnetic moments can be accounted for in terms of a coupling case between B_1 and B_2.

The ground states of the isotopes K^{39} and K^{41} have $I=\frac{3}{2}$. The odd particle (formally the proton lacking in a closed shell configuration) is expected to be in a $3d$ state. For an effective binding energy (see Section IV) of 12 Mev, one finds a value for $(R/R_0)^2_{\text{Av}}$ of 0.66. It may be noted that this value is only changed by about 1 percent if the effective binding is altered by 2 Mev.

From (18), one finds for $g_R=\frac{1}{2}$ the values $\sigma=-0.294$ and $\sigma=-0.359$ for K^{39} and K^{41}, respectively. The corresponding values of α_s obtained from (19) are -2.52 and -5.59. According to the considerations in Section V, the sign of β is negative. In fact, the spin-orbit coupling is assumed to favor large j, but the sign of this coupling is formally reversed for a particle lacking in a closed shell configuration. From (17) one thus finds

$\beta=-1.96$ and -2.46 for K^{39} and K^{41}, respectively, leading by means of (13) to the ζ values 1.02 and 0.79.

The table in **B** gives a value for b of 0.19 percent and from (15) one finally obtains

$$\epsilon(K^{39})=0.165 \text{ percent}, \quad \epsilon(K^{41})=0.396 \text{ percent}, \quad \Delta=\epsilon_{39}-\epsilon_{41}=-0.23 \text{ percent}. \tag{20}$$

The experimental value of Δ is $-(0.226\pm0.010)$ percent.

The model of the K^{39} nucleus is not quite consistent, since β is found to be slightly smaller, numerically, than the value $-(2I+1)^{\frac{1}{2}}=-2$ corresponding to a wave function for the limiting coupling case B_2. The value obtained for β corresponds to an eigenstate only if the coupling of **l** to the nuclear axis favors small values of Ω, in contradiction to the assignment $\Omega=\frac{3}{2}$ for the ground state of the nucleus.

As already mentioned, however, the choice $g_R=\frac{1}{2}$ is rather uncertain, and a slight increase of g_R suffices to make $|\beta|$ exceed 2. It may be added that even a large increase of g_R has a very small influence on Δ. For $g_R=1$, one finds $\epsilon_{39}=0.194$ percent, $\epsilon_{41}=0.432$ percent, and $\Delta=-0.24$ percent.

On the basis of the asymmetric model it thus appears to be possible to account simultaneously for the nuclear moments and for the h.f.s. anomalies of the K-isotopes.

Rb

A h.f.s. anomaly has also been observed for the Rb isotopes.[3] If, as a first approximation, these nuclei are described by the model of a single proton moving in an asymmetric nuclear core, Rb^{85} may be considered in complete analogy to the K-isotopes. For $g_R=\frac{1}{2}$, one finds $\sigma=-0.49$, $\beta=-1.7$, $\zeta=1.25$ and, $\alpha_s=-0.71$, which leads to a vanishing value of ϵ_{85}.

The magnetic moment of Rb^{87} $(I=\frac{3}{2})$ comes close to the value corresponding to the extreme coupling case B_1. For $g_R=0.8$, this coincidence would be exact; for $g_R=0.5$, a coupling case tending slightly towards A would need to be assumed. With a sufficient accuracy ζ can be obtained from (8a), giving $\zeta=0.2$. The value of α_s is close to 0.6 and is not very sensitive to the choice of g_R.

The odd particle is expected to be in a $3p$ state. For an effective binding energy of 15 Mev the value of $(R/R_0)^2{}_{\text{Av}}$ is found to be 0.49. The table in **B** gives $b=0.58$ percent, and one thus obtains $\epsilon_{87}=-0.26$ percent and, consequently, $\Delta=\epsilon_{85}-\epsilon_{87}=0.26$ percent. This value is to be compared with the empirical value of 0.33 ± 0.05 percent.

The agreement is presumably as close as could be expected since the nuclei in question may need to be considered in terms of the motion of several equivalent protons.

Other Elements

Apart from the light elements H and Li, for which the nuclear models here discussed do not apply and for which special considerations are necessary,[9] K and Rb constitute the only elements for which experimental evidence has so far been obtained regarding the effect on the h.f.s. of the intrinsic structure of the nuclear moment. Additional evidence would be of value as a further test of nuclear models.

There exist a number of other elements for which the effect, as in the two above-mentioned cases, can be determined by an accurate measurement of the h.f.s. ratio in the atomic ground state for two isotopes.

For the heavy elements, for which the h.f.s. anomaly may become very large, of the order of five percent, it may be possible to detect the effect in the h.f.s. of a single isotope if the electronic wave function can be determined with sufficient accuracy.[10]

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[9] A. Bohr, Phys. Rev. **73**, 1109 (1948); F. Low, Phys. Rev. **77**, 361 (1950).

[10] M. F. Crawford and A. Schawlow, Phys. Rev. **76**, 1310 (1949); A. Bohr and A. Schawlow (in preparation).