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Short note

Extraction of hyperfine anomalies without precise values of the nuclear magnetic dipole moment

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Abstract. A new method for extracting the hyperfine anomaly from experimental hyperfine structure constants is suggested. Instead of independent high-precision measurements of the nuclear magnetic dipole moment, precise measurements of magnetic dipole hyperfine interaction constants for two atomic states and a theoretical analysis can be used. This can lead to determination of hyperfine anomaly for radioactive isotopes where the nuclear magnetic dipole moment is not known with high accuracy.

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The influence on the hyperfine structure (hfs) of the finite size of the nucleus was considered by Bohr and Weisskopf [1]. They calculated the hyperfine interaction (hfi) of $s_{1/2}$ and $p_{1/2}$ electrons in the field of an extended nucleus, and showed that the magnetic dipole hfi constant a for an extended nucleus is generally smaller than that expected for a point nucleus. Isotopic variations of magnetic moments become larger than those in the point dipole interaction when there are different contributions to the hfs from the orbital and spin parts of the magnetisation in the case of extended nuclei. The fractional difference between the point nucleus magnetic dipole hfi constant and the constant obtained for the extended nuclear magnetisation is commonly referred to as the Bohr-Weisskopf (BW) effect [2]. The magnetic dipole hfi constant a can therefore be written as

$$a = a_{point}(1 + \epsilon_{BW}) \tag{1}$$

where ϵ_{BW} is the BW-effect, and a_{point} the a constant for a point nucleus. Because electronic wavefunctions cannot be calculated with high accuracy in complex atoms it is not possible to determine ϵ_{BW} directly; only the difference of the BW-effect in two isotopes, the so-called hyperfine anomaly (hfa), can be determined experimentally. Therefore one compares the ratio of the measured hfs constants for two isotopes (or isomers) of the same element with the independently measured ratio of the nuclear magnetic dipole moments to extract the hfa, ${}^1\Delta^2$, for the isotopes 1 and 2, and a given atomic state:

$$1 + {}^1\Delta^2 = \frac{a^{(1)}}{a^{(2)}} \frac{\mu_I^{(2)}/I^{(2)}}{\mu_I^{(1)}/I^{(1)}} \approx 1 + \epsilon_{BW}^{(1)} - \epsilon_{BW}^{(2)} \tag{2}$$

For electrons with a total angular momentum $j > 1/2$ the anomalies may be disregarded as the corresponding wavefunctions vanish at the nucleus. However, indirect influence through polarisation of the electron core [3] may give a substantial contribution to the experimental hfa [2].

The magnetic dipole hfi is normally divided into three parts [3,4], orbital, spin-orbit and contact (spin) interaction. Only the contact interaction contributes to the hfa. Thus we can rewrite the general magnetic dipole hfi constant as

$$a = a_{nc} + a_s + a_p \tag{3}$$

where a_s and a_p are the contributions due to the contact interaction of s and $p_{1/2}$ electrons, respectively, and a_{nc} is the contribution due to non-contact interactions. The experimentally determined hfa, which is defined with the total magnetic dipole hfi constant a, should then be rewritten to obtain the relative contributions to the hfa:

$${}^1\Delta^2_{exp} = {}^1\Delta^2_s \frac{a_s}{a} \tag{4}$$

and

$${}^1\Delta^2_{exp} = {}^1\Delta^2_p \frac{a_p}{a} \tag{5}$$

where ${}^1\Delta^2_s$ and ${}^1\Delta^2_p$ are the hfa for an s- or p-electron, respectively. The contact contributions a_s and a_p have to be evaluated separately by analysing the hfs. For more complex atoms with several open shells this is not a trivial task. The different contributions can only be obtained by performing an extended analysis of the hfs in several atomic states using the effective operator formalism [4]. This is, however, possible if a sufficient number of states

Table 1. Hyperfine interaction constants for Ir from [6]

	$a\ {}^{191}Ir(MHz)$	$a\ {}^{193}Ir(MHz)$	$a\ {}^{191}Ir/a\ {}^{193}Ir$	k_s	a_s/a
$5d^8 6s\ {}^4F_{9/2}$	309.410798(15)	335.289455(10)	0.9228(1)	0.1101	0.7747
$5d^7 6s^2\ {}^4F_{7/2}$	-59.9459(23)	-64.451195(18)	0.9301(1)	-0.0577	2.1122

have been measured and high-quality eigenvectors for the breakdown of LS-coupling are available. Further complications arise from the influence of core-polarisation [2] on the contact interactions, but it is still possible to do a full investigation of both the hfa and the core-polarisation by studying the experimental hfa [2]. This has been demonstrated in Eu [5], where a good consistency of Δ_s was obtained for a number of atomic states. Now it is possible to use the results from a careful analysis of the hfs to derive the hfa without exact values of the nuclear g_I factors. If we consider the hfa for two atomic states A and B in the isotopes 1 and 2 using (2), we have:

$$\begin{aligned} \frac{a_A^{(1)}}{a_A^{(2)}}\frac{g_I^{(2)}}{g_I^{(1)}} &= 1 + {}^1\Delta_A^2 \\ \frac{a_B^{(1)}}{a_B^{(2)}}\frac{g_I^{(2)}}{g_I^{(1)}} &= 1 + {}^1\Delta_B^2 \end{aligned} \tag{6}$$

Dividing these to get rid of the nuclear g_I factors:

$$\frac{a_A^{(1)}/a_A^{(2)}}{a_B^{(1)}/a_B^{(2)}} = \frac{1 + {}^1\Delta_A^2}{1 + {}^1\Delta_B^2} \tag{7}$$

Assuming that only s electrons give a contribution to the hfa in this case, we use (4):

$$\frac{a_A^{(1)}/a_A^{(2)}}{a_B^{(1)}/a_B^{(2)}} \approx 1 + {}^1\Delta_s^2\left(\frac{a_s^A}{a^A} - \frac{a_s^B}{a^B}\right) \tag{8}$$

The ratio between the two magnetic dipole hfi constant ratios for the two isotopes will be dependent only on the difference of the contact contributions of the two atomic states and the hfa for the s electron. The ratio a_s/a can be determined by the analysis of the hfs [2]. Using the effective operator formalism [4], the hfi constants can be expressed as a linear combination of effective radial parameters a_l^{ij} and angular coefficients k_l^{ij},

$$a(J) = k_l^{01}a_l^{01} + k_l^{12}a_l^{12} + k_l^{10}a_l^{10} + k_s^{10}a_s^{10} \tag{9}$$

where the indices stand for the rank in the spin and orbital spaces, respectively. The term of interest is $k_s^{10}a_s^{10}$ which is the contribution to the hfi constant from the s electron. The angular term can be evaluated if the eigenvectors of the atomic state are known. The values of the effective radial parameters are obtained by a least-squares fit to experimental hfi constants.

It should be noted that the ratio a_s/a is independent of isotopes. Once it is determined for one isotopic pair, the ratio can be used for all isotopic pairs, which is very useful in the study of hfa in radioactive isotopes. Here we demonstrate the case of Ir. The hfs of Ir has been measured by Büttgenbach et al. [6], who also performed an analysis of the hfs, where a_s^{10} was found to be 2369.1 MHz for ^{193}Ir. We consider two states, $5d^8 6s\ {}^4F_{9/2}$ and $5d^7 6s^2\ {}^4F_{7/2}$. Since they belong to different configurations the difference in the a_s/a ratio is expected to be large. The hfi constants and the angular coefficients for the contact interaction, and the a_s/a ratios are given in Table 1. The equation (8) yields ${}^{191}\Delta_s^{193}$ =0.59%, compared with the adopted value 0.64(7)% [2]. In general, it is hard to extract the error using Eq. (8) as the main error source lies in effective radial parameters and the eigenvectors. In this case, however, is the error expected to be about 25%.

It must be emphasised that the influence of the contact interaction on the magnetic dipole hfi constant, that is the level hfa, must be different between the two states used. If they are similar the difference will be small and cause an extreme sensitivity to the values used. That is the reason why the two states have to be chosen carefully. If there exist measurements of the g_I factor in stable isotopes they can be used as a calibration of this method, by determining the difference of a_s/a independently. It is then possible to use this value to determine the hfa in unstable isotopes where no or only low-accuracy measurements of the g_I factor are available. One must remember that the contact contributions to the hfs can be complicated and might give rise to unexpected errors. It is, therefore, desirable to use an independently determined hfa as calibration before making comparisons over isotopic chains.

A new method of extracting hfa is presented. The method is based on precision measurements of the magnetic dipole hfi constants and atomic calculations or careful analysis of the hfs can provide values of the hfa without precise measurements of the nuclear g_I factor. This would be very useful in determining the hfa for unstable isotopes which is of interest from nuclear-structure viewpoint.

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