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Nuclear moments: recent developments

Nicholas J. Stone [1]

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Abstract
The author has for many years kept a watching brief on the experimental study of nuclear electro-magnetic moments. Accurate values of nuclear magnetic dipole and electric quadrupole moments are a major product and the life blood of hyperfine interaction studies and their manifold applications. This paper outlines recent changes in the type of moment measurements being undertaken and the effect of modern complex electronic configuration computation on the extracted moment values.

Keywords Nuclear magnetic dipole moment · Electric quadrupole moment · Diamagnetic correction · Electric field gradient · Electro-magnetic nuclear moment data tables and recommended values

1 Introduction

It is close to thirty years since I accepted an invitation from Richard Mayer to undertake bringing the nuclear electro-magnetic moment table up to date following the 1989 listing by Raghavan [1]. Subsequently tables containing compiled references were published in 2004 and 2011 and the 2011 version was used by Mertzimekis [2] to set up the IAEA on-line nuclear electro-magnetic moment database in 2016. The most recent tables are IAEA publications [3–5]. These give single recommended values for each quantity and the same data have been incorporated in the database with fully updated lists of all references.

This short paper describes developments in the field of nuclear moments in recent years. Topics are, on the experimental side, the changing profile of new results as older facilities are closed, with the emergence of large laser-based groups at isotope separator facilities as the major source of new results and a much-reduced flow of data on short-lived states. Enhanced computation techniques are now making important contributions in both the area of electric field gradient calculations allowing extraction of improved electric quadrupole moments and in providing a new level of knowledge of diamagnetic corrections to magnetic dipole moments.

✉ Nicholas J. Stone
nick.stone@physics.ox.ac.uk

[1] Department of Physics, University of Oxford, Parks Road, Oxford, OXON OX1 3PU, UK

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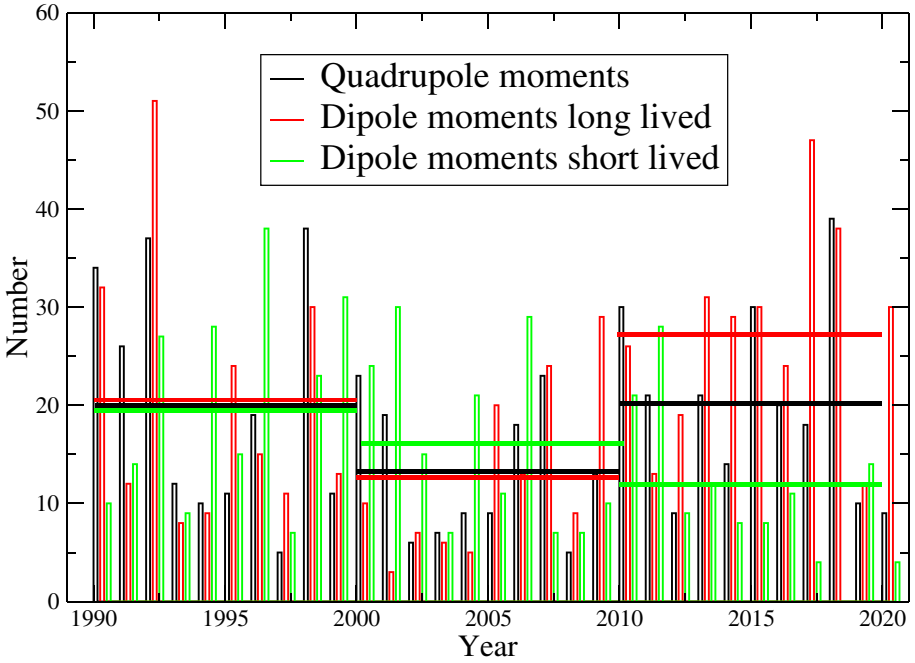

Fig. 1 Number of results by type and year. Horizontal bars represent decade averages

2 What is being measured?

Figure 1 shows the number of results now listed as recommended values for magnetic dipole moments of long-lived ($\geq$ 1 ms) and short-lived nuclear states and of nuclear electric quadrupole moments by year of publication over three decades from 1990 to 2020. The data show that for the first decade the average numbers in each category were all close to 20 per annum. Many techniques are represented both for long and short-lived states. After 2010 the numbers tell a very different story. Although the total number of results in the third decade remains close to 600 the number of measurements by the integral and time dependent angular correlation/distribution techniques fell close to zero and the total for short-lived states by close to 50%. This reflected the rapid fall in the number of groups working in this area and the closure of many smaller facilities which supported such work. New results are dominated by work on broad isotopic ranges of long-lived states which are produced by the several large groups using sophisticated laser-based techniques working at isotope separators such as ISOLDE, CERN. The field is in dire need of new initiatives yielding short-lived state moments. Ideas involving sophisticated detector arrays with complex sources exist. These aim to measure attenuation of correlations through hyperfine interactions in recoiling ions. Such experiments can utilise fission sources but require extended data taking and complex analysis.

2.1 Nuclear dipole moments

The latest ISOLDE group publication on the sequence $^{112-133}$Sb [6] exemplifies these developments. It gives results for magnetic dipole and electric quadrupole moments of 19 ground

and isomeric states. Its appearance has personal echoes for me as one who had been involved with measurements on most of the heavier Sb isotopes over a long period using the technique of NMR on Oriented Nuclei (NMR/ON). The new results show no major discrepancies with existing dipole moment data but many of the quadrupole moments are measured for the first time.

What is most appealing from the nuclear data point of view concerning the new data is that the whole sequence of isotopes was measured over a limited time in a single sequence using the same equipment. This avoids potential systematic differences which can make the assessment of the work of different groups using different methods and equipment, or even a single group over a period of years, problematic. As compared to the older NMR/ON data for which the results depended on a measurement of the hyperfine field at an Sb ion implanted into iron, known only to about 1%, the new data gives results by ratio with data taken in the same experiment on stable ^{123}Sb for which the magnetic dipole moment is claimed to be known to better than 0.1%. Thus magnetic dipole moments for the other measured states are achieved with errors smaller by an order of magnitude than previous results.

Which raises the question; how was the referenced ^{123}Sb dipole moment determined? The value taken by [6] is +2.5457(12) n.m. from Ref. [3]. This value originates from the NMR result of Proctor and Yu [7] who give a moment of 2.5341(4) n.m. based on the ratio of the ^{123}Sb resonance to that of ^{2}D in the same magnetic field. The raw experimental data requires correction for diamagnetic effects in the Sb and D (deuteron) chemical forms used but Proctor and Yu regarded the knowledge of the corrections as inadequate at that time and their results were published without correction. The correction, by close to 0.5%, applied to reach the value adopted by Lechner et al. requires explanation.

The calculation of the degree to which complex chemical electronic configurations react to screen an applied magnetic field and reduce its magnitude at a nucleus, the diamagnetic correction σ, is not simple. An early estimate of the effect in atoms was made by Lamb [8]. Later Dickinson [9] made Hartree theory calculations for atoms which gave the moment adjustment required, $(1+\sigma)$, as 1.0052 for Sb. This was adopted, with an estimated uncertainty of 5%, by Fuller [10] in her comprehensive nuclear moment and method listing of 1976. The Dickinson corrections were found to be too small by Lin, Johnson and Feioch (LJF) who made Hartree-Fock calculations (later published in expanded form [11]) for neutral atoms with result $(1+\sigma) = 1.00642$ for Sb. This value was taken by Raghavan [1] but no uncertainty in the correction was allowed for.

In the last 20 years multi-electron configuration calculations have advanced in sophistication and considerable effort has been made to improve our knowledge of diamagnetic correction factors (also known as chemical shifts) in many systems. As discussed in the preamble to Refs. [3, 4] the improved calculations are closer to the Dickinson than the LJF values. Considering data for all elements for which there have been specific modern calculation the best estimate of the correction where there has been no recent calculation is σ=0.75(10)σ_{LJF}. Hence the value $(1+\sigma) = 1.00481(48)$ for Sb applied giving the recommended value of the ^{123}Sb dipole moment. N.B. the adopted moment of ^{2}D has also been revised resulting in a further small adjustment in the ^{123}Sb dipole moment value.

2.1.1 Other diamagnetic correction developments

As mentioned above modern calculations had provided improved diamagnetic corrections applicable to magnetic dipole moments of 29 elements by the date of preparation of [3, 4]. These are calculations specific to the chemical environments in which the measurements were made. The results show decisively that the many examples of apparently discrepant,

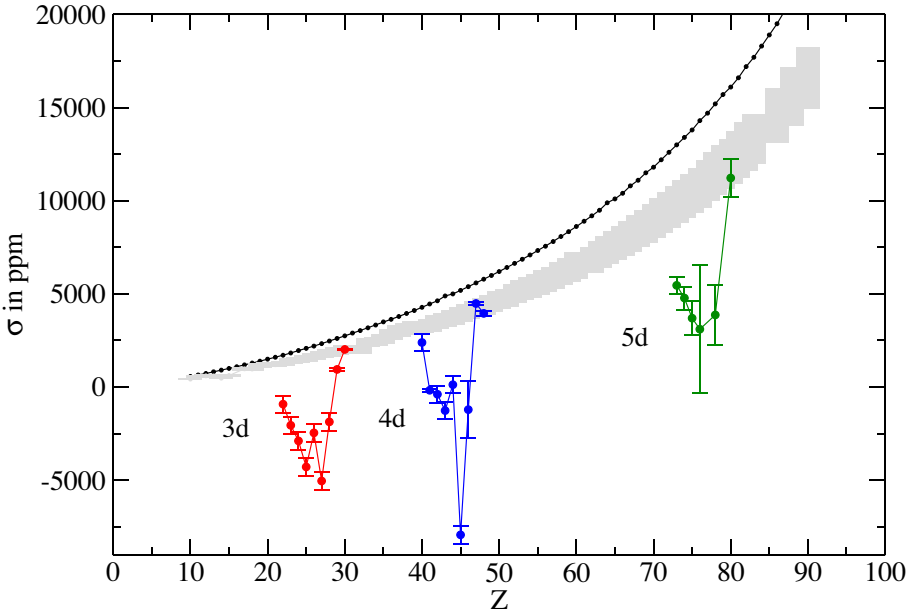

Fig. 2 Applied field correction factor as a function of atomic number Z. Black dots: LJF correction as adopted by Raghavan [1]. Grey shaded: correction with uncertainty as adopted by Stone [3, 4]. Coloured dots: correction for 3d, 4d, 5d elements calculated by Antusek and Repisky [12]. For details see text

extremely precise, magnetic dipole values presented in older tabulations resulted from the different chemical systems in which the measurements were made, with associated different corrections. What of the remaining 70+ elements?

In 2020 Antusek and Repisky [12] published the first sophisticated calculation for transition metals covering the 3d, 4d and 5d elements (Fig. 2). Their results revealed that in the chemical systems used for accurate moment determination for these elements the application of a magnetic field not only produced diamagnetic reduction of the field at the nucleus but also acted to induce a small paramagnetic moment which enhances the field. The latter effect, which had hitherto been neglected, much reduced the overall screening and, in several cases gave overall field enhancement. These new findings, with their estimated uncertainties, provide new magnetic dipole moments for all stable isotopes taken as reference moments for these elements and resolved many discrepancies in the literature. Although the changes are less than 1% in the great majority of cases, because they affect the values of stable ground state moments taken as reference values in e.g. laser spectroscopic measurements, they necessitate adjustment of both magnitude and error for the moments of many states.

For the remaining elements the estimated correction, with associated uncertainty, as described above for the example of Sb, is the best we have.

2.2 Electric quadrupole moments

The currently accepted values of nuclear electric quadrupole moments have also been strongly influenced by advances in computation which have produced more changes in recent years than any experimental development. The reason is that the measured quadrupole interaction

is the product of the moment eQ with the electric field gradient at the nucleus, usually written as *eq* ; the latter cannot be measured directly but must be calculated. Improved calculation of *eq* in atoms, ions, molecules and metals has changed the quadrupole moment values extracted from quadrupole interaction measurements by considerable factors. For the last twenty years or so Pyykko has published a series of papers reporting on these developments and offering 'reference values', usually for ground states of stable isotopes [13–15]. Using these reference values, techniques such as laser spectroscopy, which yield ratios of quadrupole interactions, can obtain quadrupole moments for different isotopes and excited states. The recent laser spectroscopy study of antimony isotopes once more offers an excellent example of how the accepted Sb quadrupole moments have been dramatically changed by the recent developments. New *eq* calculations have led to a revision far greater than any experimental result. As described by Pyykko in his 2008 paper [14], until 2006 the ground state quadrupole moment of ^{121}Sb was taken to be Q(^{121}Sb) = - 0.36(4)b based on atomic and molecular spectroscopy and old *eq* calculations. In that year two new molecular *eq* results led to revision of the moment to Q(^{121}Sb) = - 0.543(11)b, an increase of 51% in that value and all others determined from it by ratio, as in the recent ISOLDE group study.

3 Conclusion

The contraction of activity involving short-lived state nuclear moments is to be regretted as it denies theory the detailed information which knowledge of energy, spin and parity of a state cannot provide. For longer-lived states the laser techniques find ways to work with weaker beams and more complex excitations and the development of in-source ionisation methods is encouraging. Regarding electric quadrupole moments the ^{121}Sb example described is not alone and there have been major value adjustments for other elements in recent years. Quadrupole moments of V, Pm, Pb (60%) and Am have uncertainties of more than 10% and at this time there remain a further seventeen elements, Si, P, Ar, Ag, Cd, Te, Ce, Ce, Tm, W, Pt, Tl, Po, At, Cm, Bk and Cf which have no sound 'modern' *eq* calculation and hence no reference moment is established. There is clearly much work to be done.

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Author Contributions There is only one author and, he contributed 100%

Data Availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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