A-priori calculations of hyperfine interactions in highly ionized atoms: g-factor measurements of pico-second states populated in nuclear reactions.

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Abstract. Calculations of hyperfine interaction strength and life-times of states in highly ionized atoms, using the GRASP atomic structure package are reported. The calculations aim at providing calibration at Recoil-in-Vacuum nuclear excited states g-factor measurements. The method is outlined and results compared with experiment. Inclusion of decay of higher electronic states is discussed.

Keywords

Introduction

The recoil-in-vacuum [RIV] method uses attenuation of gamma-ray angular distributions from aligned nuclear systems such as are created, for example, in Coulomb excitation, to measure excited state g-factors. The method has been shown, in an experiment on the first 2^+ state of ^{132}Te, to offer attractive possibilities for application with relatively weak radioactive ion beams [RIBs] when combined with modern detector arrays [1]. In that measurement the magnetic hyperfine interaction acting on the nuclei of the recoiling ions was calibrated using 2^+ states of other Te isotopes having known lifetime and g-factor. However the attenuation is a function of nuclear state spin and for most elements and for other than first 2^+ states, no suitable calibration states exist.
It is of clear importance to establish how the interaction varies with element and ionization state in order that the RIV method may be applied to a wide range of isotopes and to states of differing nuclear spin. This paper describes an attempt to calculate the interaction from first principles using the GRASP2K fundamental atomic physics theory [2]. The calculation, which has been applied to systems ranging from 5-electron Fe ions to 23-electron Te ions, is briefly described. The results, compared with recent RIV experiments, show great promise that such calculations can provide parameter free, a-priori, calibrations for RIV experiments. Important questions concerning the treatment of short-lived electronic excited state are discussed. The calculations are readily adapted to any nuclear level spin, allowing extension of measurement beyond the usual 2^+, (4^+) states of even-even isotopes to levels in odd-A and odd-odd isotopes. In addition to Coulomb excitation, experiments on fusion reactions and fission fragments are outlined.

A-Priori calculation of the magnetic hyperfine interaction in highly ionized atoms.

The steady development of computing power and methods of calculation of hyperfine interactions of multiply ionized atoms now make possible a radically different and more general approach to RIV calibration, namely the derivation of the atomic physics of the attenuation from first principles. This fundamental approach requires detailed knowledge of the contributing *J* states, their magnetic hyperfine interaction strengths *A(J)* and the relative

probabilities of the ionic charge states present in the recoil ion population. Pioneer attempts at such calculations have been made in the past for light elements [3, 4] but this is the first approach to such a calculation valid for a wide range of elements and charge states.

The calculation uses the Dirac-Hartree-Fock multi-configuration model coded as the GRASP package built up over the years by the groups at Oxford and Vanderbilt University and their collaborators. A full description can be found in Ref. [2].

The ionic charge states present in the emerging ions recoiling from the target, and their relative probabilities, have been calculated using the EQFOIL code by D. E. Hoglund (1984) available at the HRIBF facility, Oak Ridge, based on the known beam energies and target thicknesses.

We consider experiments in which the attenuations measured are not functions of time, but are integrated over the nuclear state lifetime. At this stage we assume that the electronic states live longer than the nuclear lifetime (the static model) , but see later remarks. The attenuation factors G_k form part of the expression for the angular distribution

$$W(\theta_\gamma,\phi) \approx \sum_{k.q} G_k \rho_{kq} A_k Q_k D_q^{k*}(\phi,\theta_\gamma,0) \qquad (1)$$

where all parameters have their usual meanings [5, 6] and G_k are the g-factor dependent attenuation coefficients, obtained by comparison of the distribution measured in recoiling ions to the un-attenuated distribution. The latter can be calculated using Coulomb excitation theory [6] and/or, for non-radioactive beams, measured when the recoils are stopped in a metal in which they rapidly neutralize, eliminating the attenuation process.

The attenuation factors G_k are functions of the angular momenta involved, the precession frequencies, and time. When the integrated attenuation over the nuclear lifetime τ is measured, rather than the time dependence of the attenuation, this lifetime becomes the time parameter of the measurement. In this paper we consider the scenario in which the electron interaction remains constant over the nuclear state lifetime, the so-called 'static model' of the interaction discussed by Frauenfelder and Steffen [5]. Extension of the present work to include the possibility of electronic transitions during the attenuation process is outlined in the discussion. For this model the G_k coefficients are given by:

$$G_k(\infty) = \sum_{F,F'} q(J) \frac{(2F+1)(2F'+1)}{2J+1} \begin{Bmatrix} F & F' & K \\ I & I & J \end{Bmatrix}^2 \frac{1}{(\omega_{F,F'}\tau)^2+1} \qquad (2)$$

The hyperfine splittings are given by

$$E_F = A(J)\mathbf{I}.\mathbf{J} = A(J)[F(F+1) - J(J+1) - I(I+1)]/2 \qquad (3)$$

and the precession frequencies by

$$\omega_{F,F'} = \frac{\pi}{h} A(J)[F(F+1) - F'(F'+1)] = \frac{2\pi}{h} A(J)F \qquad (4)$$

The G_k calculation considers each contributing ionic charge state separately. For each charge the states deriving from low-lying electronic configurations are analyzed in GRASP2K to give their total angular momentum *J*, binding energy and magnetic hyperfine interaction parameter, *A(J)*. Using the *A(J)* parameters, values of G_k are calculated for each *J* state, for a specific nuclear spin *I*, as a function of nuclear lifetime and g-factor using Eqs. (2, 4).

Many *J* states are involved. To conclude the calculation two important decisions must be taken. The choice of configurations to be included in the calculation for each charge state has been made on the basis of excitation energy above the ground state configuration. Increasing energy relates to decreasing lifetime of the states associated with a given configuration. To be of concern to the experiment the excited electronic state lifetime must be sufficient to produce

an appreciable precession of the nuclear spin. Since the *A(J)* parameters are < ~ 10^5 MHz (for a nuclear g-factor of ~ 0.5), at a first estimate all states of lifetime shorter than ~ 10^{-14} s can be safely neglected. In hydrogen an allowed E1 atomic transition of energy E ~ 10 eV has lifetime ~ 10 ns. With transition probability proportional to E^3, an excited state of lifetime ~ 10^{-14} s will be at excitation energy ~ 1000 eV: this energy has been taken to limit the excitations to be included. Each configuration produces states having a spread of excitation of typically 100-200 eV, with all *J* values well mixed within this range so all states for a selected configuration have been included. The calculation shows clearly the energy cost of exciting individual electrons to higher sub-shells. Thus holes in lower principal quantum number, *n*, 'core', sub-shells, filled in the ground state, i.e. $n = 1$ in ionised Ge and $n = 1,2$ in ionized Mo, are of too high energy and too short-lived to contribute to the observed attenuations.

The second decision concerns the weight to be given to each state. For each configuration the relative weight of each *J* state is taken as $(2J + 1)$. This follows previous attempts at a-priori calculations. For even numbers of electrons, states having $J = 0$ are included in these averages, with $A(J=0) = 0$. This weight assignment is consistent with the random production of the electronic states as the ions leave the target, giving equal a-priori probability to the $(2J + 1)$ magnetic substates of each *J* state. Previous studies have reported experimental evidence for departure from this weighting. The ability of the present calculation to deal with departures from the $(2J + 1)$ weighting is further discussed below.

With this energy selection and electronic state weighting the average G_k factors for any system may be calculated. There are no other adjustable parameters in the calculation.

Comparison with experiment.

As an example we show in Fig. 1 comparison between calculation and experiment for some Mo, Ru and Pd first 2+ states having well known g-factors and lifetimes. The figure shows the individual calculation for various contributing charge states (solid lines) as well as the final average result (heavy dotted lines). The agreement between experiment and theory is very satisfactory.

Fig 1. Attenuations measured for Mo, Ru and Pd isotopes compared with calculation.

Application of the theory

The availability of a microscopic theory of the attenuation opens important new opportunities to experimenters. It becomes simple to make adjustment of the calibration for variation of the nuclear spin of the Coulomb excited state. This is illustrated in Figure 2 for the case of a 15 electron Mo ion and I = 2, 4 and 10. The figure demonstrates that although increasing nuclear spin leads to decreased sensitivity of the RIV method the G_4 attenuation factor in particular can remain useful to relatively high spin values.

The most fundamental development is that attenuation measurements on all accessible nuclear states, from even-A and odd-A nuclei alike, can be interpreted to yield nuclear parameters without the necessity that g-factors and lifetimes of similar states be available for calibration. This offers a major advance. g-factors of excited states in odd-A isotopes have great potential interest as revealing single-particle make-up of the states, whereas those of 'collective' even-even excitations have limited range and interest.

Fig. 2. Attenuation factors G_k for 15 electron ^{98}Mo ions with nuclear spin $I = 2.4$ and 10.

In making comparison with nuclear theory it is usual to consider lifetimes τ and g-factors of excited states as separate entities. However theory makes prediction of both these parameters, and so also of their product. Experiments giving values of the product $g\tau$ are thus good tests of theory even when they are not separated. Fig. 3 shows the attenuations expected, based on predicted values of the $g\tau$ product, for excited states in ^{129}Sb [7]. The G_k curves in the figure are calculated for Te ions and for nuclear states of spin 2, which will be close to those for Sb ions of similar energy. The figure illustrates the fact that, although the range of $g\tau$ for which the RIV method has sensitivity is limited, measurements on many excited states should lie within the useful range of the method.

Fig 3. Predicted attenuations for a series of excited states in ^{129}Sb, based on shell-model calculations of their $g\tau$ values.

Beyond the $(2J + 1)$ state weighting.

The a-priori calculation provides lifetimes of each J state. This the mean turn angle though which a nuclear spin will precess whilst in each J state is a feature of the model. Also the lower state to which any state will decay is known. Where the lifetime is short and the turn angle small the model is easily improved by considering the weight of the initial state to be passed down to the lower state. This modification of the model is of particular relevance when there are a group of low lying states fed by higher-lying short-lived states with an energy gap, such as occurs if the lower states involve electrons in the n = 2 major shell, with excited states involving promotions to n = 3. An example of calculation in which this has been done is shown in Fig. 4 for 5electron Fe ions. It is seen that the basic $(2J + 1)$ model gives poor agreement with experiment, but that allowing for decay improves the agreement.

Fig. 4. Model calculations for 5-electron Fe ions with and without considering higher state decay, compared with experiment.

Discussion

The first applications of the a-priori calculations described in this paper show encouragingly good agreement with experiment. It is clear that more complete testing of the theory is required before its general applicability, with good precision, can be assured. Such tests are in progress. Since the calculations provide lifetimes of the excited electronic states, detailed investigation of the assumption that the interaction is ‘static’ during the nuclear lifetime becomes possible for the first time. Decay of the more excited electronic states not only eliminates some from the averaging process, but also affects the weighting of the longer lived states.

Coulomb excitation is not the only means to provide a source of aligned recoiling nuclei. Although little investigated, it is known that fission produces planar alignment of fragment nuclear spins. With sophisticated arrays for fission fragment and gamma ray detection, fission sources may offer another substantial area of application of RIV and these calculations.

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Fig.1

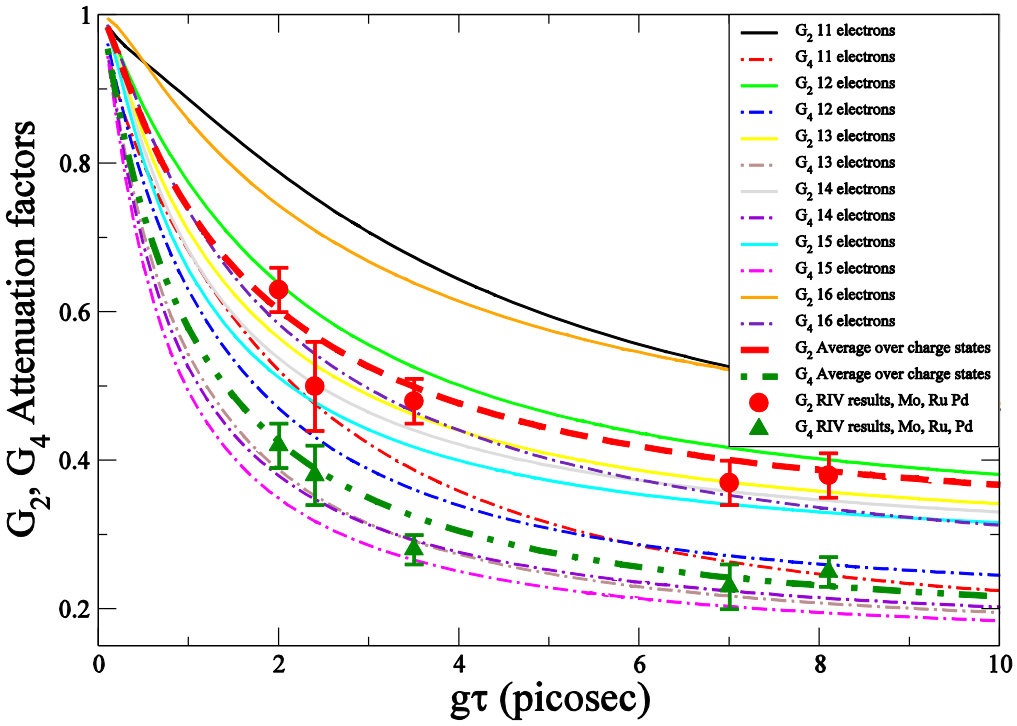

G2, G4 Attenuation factors
gτ (picosec)
G2 11 electrons
G4 11 electrons
G2 12 electrons
G4 12 electrons
G2 13 electrons
G4 13 electrons
G2 14 electrons
G4 14 electrons
G2 15 electrons
G4 15 electrons
G2 16 electrons
G4 16 electrons
G2 Average over charge states
G4 Average over charge states
G2 RIV results, Mo, Ru Pd
G4 RIV results, Mo, Ru, Pd

Fig.2

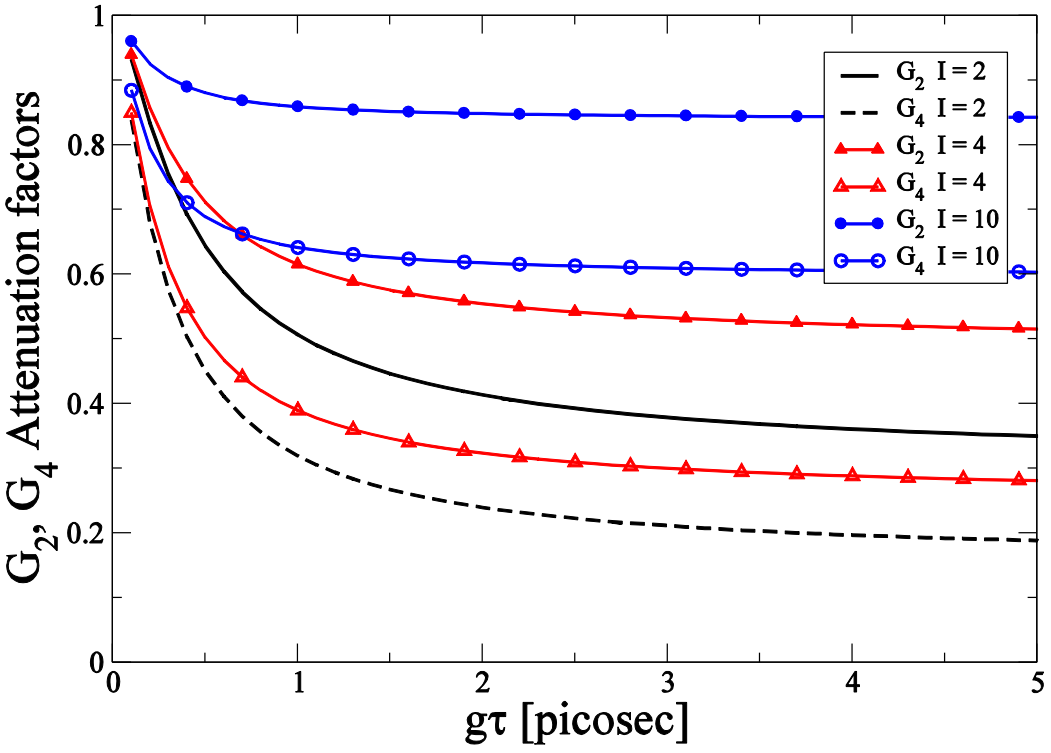

G2, G4 Attenuation factors
gτ [picosec]
G2 I = 2
G4 I = 2
G2 I = 4
G4 I = 4
G2 I = 10
G4 I = 10

Fig.3

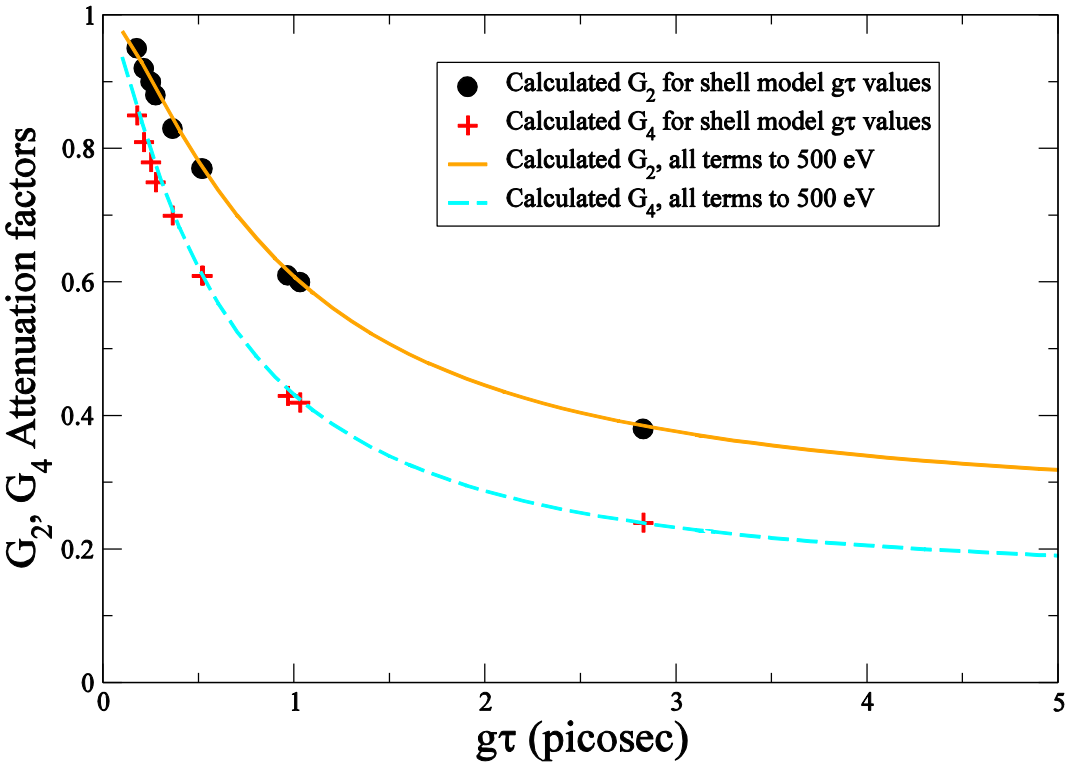
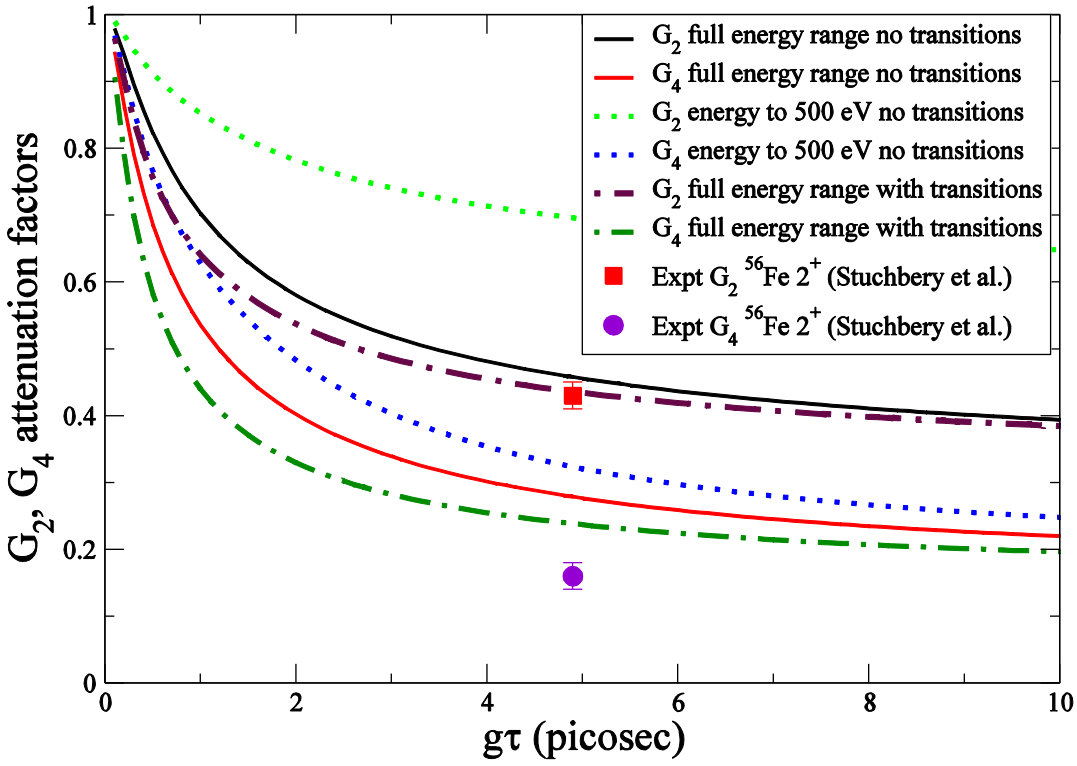

Calculated G_2 for shell model gτ values
Calculated G_4 for shell model gτ values
Calculated G_2, all terms to 500 eV
Calculated G_4, all terms to 500 eV
G_2, G_4 Attenuation factors
gτ (picosec)
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5

Fig.4


G_2 full energy range no transitions
G_4 full energy range no transitions
G_2 energy to 500 eV no transitions
G_4 energy to 500 eV no transitions
G_2 full energy range with transitions
G_4 full energy range with transitions
Expt G_2 ^{56}Fe 2^+ (Stuchbery et al.)
Expt G_4 ^{56}Fe 2^+ (Stuchbery et al.)
G_2, G_4 attenuation factors
gτ (picosec)
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10