

PhD Thesis

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## Accepted papers

- [1] B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum. Calculation of atomic spectra and transition amplitudes for superheavy element Db ( $Z=105$ ). *Physical Review A*, 98:022518, 2018
- [2] B. G. C. Lackenby and V. V. Flambaum. Weak Quadrupole Moments. *Journal of Physics G*, 45:075105, 2018
- [3] B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum. Atomic structure calculations of superheavy noble element oganesson ( $Z=118$ ). *Physical Review A*, 98:042512, 2018

## Part I

# Second order tensor properties in deformed nuclei

# Chapter 1

## Background Information

### 1.1 Nuclear Units

In this thesis we will use the framework of nuclear units. In this framework we set  $\hbar = c = 1$ .

- included cited discussion on the concept of using low energy detection to detect high energy phenomena.

### 1.2 Parity nonconservation in atomic systems

The standard model has stood the test of time coming out on top time again after countless tests. Detection of the violation of fundamental symmetries is an avenue which is suspected to overthrow the model by suggesting a deeper underlying theory. It is suspected that the standard model is a low energy approximation to a more fundamental theory of the universe similar to how classical physics is a large spacial approximation to quantum theory. There are a number of discrete symmetries which form the basis of our current interpretation of the universe. They are time-reversal  $T$  parity and charge conjugation (get the paragraph from Honours thesis).



Of these discrete symmetries only parity has been determined to be violated. This is a prediction of the standard model weak interaction and therefore the bubble has yet to burst on the standard model. In this thesis we will look at some processes which violate these symmetries.

### 1.3 CPT Theory

A cornerstone of modern quantum field theory is the CPT theorem. In essence it states that all physical phenomena are CPT-even which means under the application of the three operators the system is unchanged. [?]

### 1.4 Collective Properties of Nuclei

A major focus of this thesis is the enhancement of nuclear properties in non-spherical (or deformed) nuclei. It has been known for nearly a century that some nuclei are non-spherical. Experimental confirmation of deformed nuclei came with the measurement spectroscopic electric quadrupole moment of the nucleus by Th. Schuler in 1936 [Add reference]. Theoretical study was backed up by Casimir in his works [Casimir citations]. The electric quadrupole is a second order tensor defined as the non spherical distribution of electric charge in the nucleus. As neutrons are uncharged this moment is just the distribution of protons.

- Included discussion of possible nuclear models.
- Included in depth discussion of the Nilsson model with positives and negatives
- Discussed why first order tensor properties such as magnetic moments are not collective properties but second order tensors are.
- Included discussion on the high angular momentum states

- included distinction between the intrinsic frame of the nucleus (rotating frame) and the laboratory frame of the nucleus. Included the tensor relationship between the rotating and laboratory frame.

## 1.5 Lorentz Violation and Extension of the Standard Model

It is well known that the vacuum speed of light is constant and the cosmic speed limit which was famously first proposed by Einstein in 19\*\* in his theory of special relativity. For the past century this theory has had unparalleled success with no suggestion of failing. The basis of special relativity is the invariance of Lorentz symmetry.

Lorentz Symmetry is a fundamental symmetry which in essence states that there is not preferred reference frame of the universe and that the laws of physics are unchanged when the orientation of the system (rotation) or speed of the system (boosts) is changed. It is one of the most fundamental symmetries of physics. However modern physics suspects that it will not always be conserved and that, like other symmetries, Lorentz invariance is a low energy property of the universe but can be broken in high energy theories.

Tests of Lorentz invariance date back to the famous Michelson and Morley experiment in the late 19th century [?] which returned a null result (Confirming there is no lumeriferous ether and also verifying Lorentz symmetry).

Due to its fundamental importance in the current standard model of particle physics all interactions must conserve Lorentz symmetry.

## 1.6 Neutron Quadrupole moment

The deviation of density from a spherical symmetry is known as the quadrupole moment. The spectroscopic moment along the  $z$ -axis of the nucleus is given by,

$$Q_{zz} = e \sum N (2z^2 - x^2 - y^2)$$

where specifically the electric quadrupole moment which is the cahрге deviation from spherical symmetry is given by,

$$Q_e = eQ_{zz}$$

- Compared to proton quadrupole moment.
- include mathematical descritpion including charge and density.
- Discuss connection to Weak charge and PNC
-

## Chapter 2

# Calculations

### 2.1 Splitting of energy bands in deformed nuclei

In the Nilsson model the energy levels are split due to the

### 2.2 Lorentz violating parameters in nuclei

### 2.3 Quadrupole moments of neutrons in nuclei

### 2.4 Magnetic quadrupole moment in deformed nuclei

TP violating nuclear moments induce a spin hedgehog wavefunction.

$$|\psi'\rangle = \left(1 + \xi \hat{\boldsymbol{\sigma}} \hat{\mathbf{V}}\right) |\psi_0\rangle$$

where  $|\psi_0\rangle$  is the unperturbed wavefunction. The magnetic quadrupole moment of the nucleus (MQM) is defined by the second order tensor operator,

$$\hat{M}_{kn} = \frac{e}{2m} \left[ 3\mu \left( r_k \sigma_n + \sigma_k r_n - \frac{2}{3} \delta_{kn} \hat{\sigma} \mathbf{r} \right) + 2q (r_k l_n + l_k r_n) \right]$$

for the unperturbed wavefunction the matrix element vanishes  $\langle \psi_0 | \hat{M}_{kn} | \psi_0 \rangle = 0$ . However after it is perturbed by the TP odd interaction there is a non zero matrix element.

$$\begin{aligned} M_{kn} &= \langle \psi' | \hat{M}_{kn} | \psi' \rangle \\ &= \langle \psi_0 | \hat{M}_{kn} | \psi_0 \rangle \\ &\quad - \xi \langle \psi_0 | \left[ \hat{\sigma} \hat{\nabla}, \hat{M}_{kn} \right] | \psi_0 \rangle \\ &\quad - \xi^2 \langle \psi_0 | \hat{\sigma} \hat{\nabla} \hat{M}_{kn} \hat{\sigma} \hat{\nabla} | \psi_0 \rangle \end{aligned}$$

as stated above the first term vanishes also ignore the last term as it is heavily suppressed due to  $\xi^2$  the MQM due to the TP violating effects is given by the matrix element,

$$M_{kn} = -\xi \langle \psi_0 | \left[ \sigma_\nu \nabla_\nu, \hat{M}_{kn} \right] | \psi_0 \rangle$$

This simplifies to 4 effective matrix elements,

$$\begin{aligned} M_{kn}^{(1)} &= \langle \psi_0 | \sigma_m \nabla_m \left( r_k \sigma_n + \sigma_k r_n - \frac{2}{3} \delta_{kn} \sigma_\nu r_\nu \right) | \psi_0 \rangle \\ M_{kn}^{(2)} &= \langle \psi_0 | \sigma_m \nabla_m (r_k l_n + l_k r_n) | \psi_0 \rangle \\ M_{kn}^{(3)} &= \langle \psi_0 | \left[ \sigma_m, r_k \sigma_n + \sigma_k r_n - \frac{2}{3} \delta_{kn} \sigma_\nu r_\nu \right] \nabla_m | \psi_0 \rangle \\ M_{kn}^{(4)} &= \langle \psi_0 | [\sigma_m, r_k l_n + l_k r_n] \nabla_m | \psi_0 \rangle \end{aligned}$$

These 4 matrix elements will determine the MQM in nuclei. We will go through each of the matrix elements separately. The first element,

$$\begin{aligned} M_{kn}^{(1)} &= \left\langle \sigma_m \nabla_m \left( r_k \sigma_n + \sigma_k r_n - \frac{2}{3} \delta_{kn} \sigma_\nu r_\nu \right) \right\rangle \\ &= \left\langle \sigma_m \left( \delta_{km} \sigma_n + \delta_{mn} \sigma_k - \frac{2}{3} \delta_{kn} \delta_{m\nu} \sigma_\nu \right) \right\rangle \\ &= \left\langle \sigma_k \sigma_n + \sigma_n \sigma_k - \frac{2}{3} \sigma_\nu \sigma_\nu \right\rangle \end{aligned}$$

Using the Pauli matrices properties for the anticommutator and product we have  $\{\sigma_k, \sigma_n\} = 2I_2 \delta_{kn}$  and  $\sigma_\nu \sigma_\nu = 3I_2$  therefore we have that,

$$M_{kn}^{(1)} = 2I_2 \delta_{kn} - \frac{2}{3} 3I_2 = 0.$$

The second matrix element is given by ,

$$\begin{aligned} M_{kn}^{(2)} &= \langle \sigma_m \delta_m (r_k l_n + l_k r_n) \rangle \\ &= \langle \sigma_m [\delta_{km} l_n + \delta_{nm} l_k] \rangle \\ &= \langle \sigma_k l_n + \sigma_n l_k \rangle \end{aligned}$$

The third matrix element is given by,

$$M_{kn}^{(3)} = \langle [\sigma_m, r_k l_n + l_k r_n] \nabla_m \rangle$$

as  $r_i, l_j$  and  $\sigma_k$  commute for  $i, j, k$  we have that,

$$M_{kn}^{(3)} = 0.$$

For the last matrix element we have,

$$\begin{aligned}
M_{kn}^{(4)} &= \left\langle \left[ \sigma_m, r_k \sigma_n + \sigma_k r_n - \frac{2}{3} \delta_{kn} \sigma_\nu r_\nu \right] \nabla_m \right\rangle \\
&= \langle [\sigma_m, r_k] \sigma_n \nabla_m + r_k [\sigma_m, \sigma_n] \nabla_m + [\sigma_m, \sigma_k] r_n \nabla_m \\
&\quad + \sigma_k [\sigma_m, r_n] \nabla_m - \frac{2}{3} \delta_{kn} [\sigma_m, \sigma_\nu] r_\nu \nabla_m \rangle \\
&= r_k [\sigma_m, \sigma_n] \nabla_m + r_n [\sigma_m, \sigma_k] \nabla_m - \frac{2}{3} \delta_{kn} [\sigma_m, \sigma_\nu] r_\nu \nabla_m
\end{aligned}$$

Using the Pauli commutation relations  $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$  we have that,

$$M_{kn}^{(4)} = \langle 2ir_k \epsilon_{mna} \sigma_a \nabla_m + 2ir_n \epsilon_{mka} \sigma_a \nabla_m \rangle - \frac{2}{3} \delta_{kn} 2i\epsilon_{m\nu a} \sigma_a r_\nu \nabla_m$$

We can rewrite this as,

$$M_{kn}^{(4)} = r_k B_n + r_n B_k - \frac{2}{3} \delta_{kn} r_\nu B_\nu$$

where  $B_i = 2i\epsilon_{mia} \sigma_a \nabla_m$ . we are interested in the projection of the MQM on the symmetry axis of the nucleus which we will denote as the  $z$  axis. Therefore we want to find  $M_{zz}$  projection. For the non vanishing matrix elements we will find the value of the projection,

$$M_{zz}^{(2)} = \langle 2\sigma_z l_z \rangle$$

Pauli matrices are related to the spin matrices by the relation,

$$\sigma_i = 2s_i$$

and therefore the matrix element is given by,

$$M_{zz}^{(2)} = 4 \langle s_z l_z \rangle$$

For the unperturbed state we will use the Nilsson basis described in the 1955 Nilsson paper [?]  $|\psi_0\rangle = |Nl\Lambda\Sigma\rangle$ . From [?] the matrix element  $\langle s_z l_z \rangle = \langle s_z \rangle \langle l_z \rangle = \Sigma\Lambda$ .

For the other matrix element we have to simplify the matrix element first.

$$\begin{aligned}
\frac{\langle r_\nu B_\nu \rangle}{2i} &= \langle r_\nu \epsilon_{m\nu a} \sigma_a \nabla_m \rangle \\
&= -i \langle \sigma_a \epsilon_{a\nu m} r_\nu p_m \rangle \\
&= -i \langle \boldsymbol{\sigma} \cdot (\mathbf{r} \times \mathbf{p}) \rangle \\
&= -i \langle \boldsymbol{\sigma} \cdot \mathbf{l} \rangle \\
\Rightarrow \langle r_\nu B_\nu \rangle &= 2 \langle \boldsymbol{\sigma} \cdot \mathbf{l} \rangle \\
&= 4 \langle \mathbf{s} \cdot \mathbf{l} \rangle \\
&= 4\Sigma\Lambda
\end{aligned}$$

Also

Therefore the total quadrupole moment is given by,

## 2.5 Schiff moment in nuclei



## Chapter 3

# Results

## Part II

# Atomic Calculations

## Chapter 4

# The CIPT Method

The CIPT method is a multi-electron method used to calculate the spectra of atoms. It was developed by V. A. Dzuba at UNSW Sydney and employs a combination of the configuration interaction and Perturbation Theory.

### 4.1 Hartree-Fock

### 4.2 Basis States

### 4.3

## Chapter 5

# Super Heavy Elements

# Bibliography

- [1] B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum. Calculation of atomic spectra and transition amplitudes for superheavy element Db ( $Z=105$ ). *Physical Review A*, 98:022518, 2018.
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