Theoretical and experimental developments for symmetry-violating nuclear properties

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I. SCIENTIFIC ISSUE

Over the past decade a tremendous progress has been made in our understanding of ground-state nuclear properties, due to a strong collaboration between nuclear theory and precision experiments [1]. Laser spectroscopy measurements, in particular, can provide access to nuclear electromagnetic properties along isotopic chains, allowing the extraction of nuclear charge radii, magnetic dipole and electric quadrupole moments. These measurements have been critical to guide the development of nuclear theory [1–6]. On the experimental side, these achievements became possible due to improvements in laser spectroscopy technology, as well as the efficient production of radioactive, short-lived isotopes at the various radioactive ion beam (RIB) facilities world wide [1, 7–9]. In parallel, nuclear theory underwent a rapid progress due to key advancements in the development of many-body methods, the description of inter-nucleon interactions and operators based on chiral effective field theory (EFT), the use of emulators [10], as well as the increase in the available computing power [11–15]. This simultaneous progress further motivates the need for a strong collaboration between theory and experiment [1].

Very recently, experiments with radioactive molecules, in particular those containing octupole deformed nuclei, have emerged as a highly promising platform upon which to perform precision studies of electroweak nuclear properties, in particular parity (P) and/or time-reversal (T) violating nuclear moments [16]. Such measurements can provide unique access to some of the worst constrained parameters of the Standard Model (SM), allowing for precise studies of the nuclear electroweak interaction (e.g. measurements of nucleon-meson P-violating couplings, anapole moments or even weak quadrupole moments) [16, 17]. Moreover, non-zero measurements of simultaneous P- and T- violations would be a clear sign of new physics beyond the SM at the hadronic level and it could help us answer some of the biggest open questions about our universe, such as the nature of dark matter, the matter-antimatter asymmetry or the strong CP problem [16, 17]. This direction of research was significantly accelerated by the recent precision measurement of the first radioactive molecule, radium monofluoride (RaF), which proved its extreme sensitivity to minuscule nuclear effects, as well as its suitability for laser cooling and trapping, techniques paramount for performing precision studies in these systems [18–21]. This motivated major efforts at various RIB facilities world wide (e.g. CERN in Switzerland, FRIB in the US, RIKEN in Japan) in producing and studying new radioactive molecules, with potential for symmetry violating searches (e.g. molecules containing protactinium) [16].

Despite this experimental progress, very little is know theoretically about symmetry-violating nuclear properties. For light nuclei, No Core Shell Model (NCSM) calculations of the P-violating nuclear anapole moment [11] and the nuclear electric dipole moment (EDM) [12] showed promising preliminary results. However, *ab inito* calculations are

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not available yet for medium and heavy mass nuclei, including octupole deformed ones, where the biggest experimental signals are expected. Even for ^{133}Cs, where the only non-zero measurement of a nuclear anapole moment has been observed [22], no reliable nuclear structure calculations exist, despite almost 30 years since the experiment was performed. Moreover, due to the wide range of effects that can contribute to a given measurement, experiments in nuclei across the entire nuclear chart need to be performed in order to disentangle such effects [17]. Thus, calculations are needed in all nuclear mass regions and hence a wide range of techniques are needed for this field to progress. Equally important is the proper uncertainty estimation of the calculated nuclear structure parameters [13, 23, 24]. Given the complexity of future experiments, which can take years to perform, even a factor of two uncertainty in a predicted nuclear property of interest can make the difference between an experiment being feasible or not [25, 26].

The purpose of this workshop is to bring together world leading experts in the field of fundamental symmetry violations, both on the experimental and theoretical side to discuss the best directions to pursue in order to achieve a fast progress in this newly emerging field. We would like to organize the workshop in such a way that stimulating theoretical discussions can take place, motivated by the possible near and long term experimental measurements planned using radioactive molecules. A great focus will be put on the progress made using various many-body methods, their suitability for the problem at hand, and ways in which different methods can benefit from and benchmark their results with each other. We believe that this workshop is extremely timely, given the fast paced experimental progress and the need for theoretical calculations to guide and interpret such experiments.

Given the wide range of nuclei the community is interested in, the Energy Density Functional (EDF) approach continues to be a promising tool for performing such calculations [27]. Here, of great interest is the use of EDF for the calculation of pear deformations and Schiff moments in odd-even and odd-odd nuclei, which are of interest for experimental measurements [16, 28]. While work in this direction has seen progress recently, by using projection techniques for the calculations of Schiff moments [29], a lot still remains to be done. At the same time, EDF can also be use for systematic calculations of anapole moments across the entire nuclear chart, taking into account in a self-consistent manner important effects, such as these coming from the spin and orbital currents present in the nuclear core [16, 30]. The progress made, as well as future plans in these directions of research will be discussed.

In parallel to EDF, advancements made in *ab initio* calculations will also be discussed [31]. Some success has been seen in using NCSM calculations [11, 12, 32], but further improvements can be made. Currently, phenomenological one-meson-exchange potentials are used for the parity and/or time-reversal violating interactions [11, 12]. A more desirable approach would be a description based on chiral EFT, which has been recently developed [33–35]. This would allow a consistent and systematically improvable treatment of these symmetry violating interactions [16]. In addition, developments in complementary many-body methods such as In-Medium Similarity Renormalization Group (IMSRG) [36, 36, 37], Coupled Cluster (CC) [38, 39], projected generator coordinate method (PGCM) [40] or self-consistent Green's functions [41] are needed in order to extend the reach of the available calculations to medium mass and heavy nuclei [16].

A big challenge for many-body methods is the scaling to nuclei where the largest experimental signals are expected ($A \gtrsim 200$) [37, 38]. Until recently, a major issue was presented by the convergence of calculations of 3 body force matrix elements for nuclei with $A \gtrsim 100$, limited by the available computing resources. However, recently, a novel way in storing the needed matrix elements for such calculations suitable for methods that use spherical references, extended the reach of nuclear *ab initio* calculations to Sn and even to the doubly magic ^{208}Pb nucleus [13, 42]. This region is already of high interest for parity violation studies [16, 17]. The study of ^{208}Pb neutron skin also showed the power of using machine learning and statistical methods applied to nuclear calculations in order to predict reliable uncertainties on the calculated parameters [13]. However work still needs to be done for nuclei with strong quadrupole and octupole deformations, in the light actinide region, which exhibit a large sensitivity to both P- and T- violations [16, 17]. A main advantage of (statically) octupole deformed nuclei is the existence of a ground state parity doublet. Thus, unlike non-octupole deformed nuclei, where P- and T-violation calculations require in inclusion of many excited states with energies at the MeV scale and above, for octupole deformed ones, only the parity doublet is relevant for such calculations. However, the octupole deformation requires an intrinsically deformed reference state, thus shell-model based approaches won't be suitable in this case [16]. Methods built on a deformed mean-field state, able to include the collective physics in the used reference state, such as In Medium Generator Coordinate Method (IM-GCM), PGCM or coupled cluster should be a promising avenue, although works still needs to be done on extending them to heavy nuclei [13, 16, 43]. The prospects of harnessing this tremendous progress towards computing nuclear symmetry violating properties will be a main topic of discussion for this proposed workshop.

II. GOALS OF THE PROJECT

Major breakthroughs are expected in the following years on the experimental side using short-lived, radioactive molecules, in the measurements of symmetry violating nuclear properties. Accurate theoretical calculations are therefore urgently needed, together with reliable uncertainties, in order to interpret these results and lead the experimental searches towards the most promising nuclei. The main goals of this workshop are :

1. Bring together world leading experts, on the theoretical and experimental side of this field, in order to discuss the rapid progress made in the past few years, as well as the main directions to be pursued in the near future.
2. Discuss the most promising nuclei where large enhancements in the sought for signal are expected and that are suitable for experimental investigation in the next $5 - 10$ years.
3. Discuss the prospect of Energy Density Functionals to calculate nuclear Schiff moments and nuclear anapole moments across the entire nuclear chart, with a particular emphasis on the octupole deformed, light actinide region.
4. Discuss the prospect of including chiral parity- and time-reversal violating potentials, as well as two-body currents in nuclear structure calculations using *ab initio* methods.
5. Discuss the prospects of using emulators and statistical methods to provide reliable uncertainties on the values of the computed physical quantities.
6. Discuss the possibilities of applying *ab initio* methods to octupole deformed nuclei, where spherical reference states are not suitable anymore.
7. Work towards building a closer collaboration between experimentalists and theorists working in this field. The possibility of having PhD students or postdoctoral researchers from theoretical groups spend a semester in an experimental group (or the other way around) will be discussed, even the possibility of creating fellowships able to facilitate such much needed exchanges.

III. CONFIRMED SPEAKERS

Experiment

— Pierre Delahaye (GANIL), "Searching for CP violation in the radioactivity of polarized ions : The MORA project"
— Ronald Fernando Garcia Ruiz (MIT), "Fundamental Physics Studies with Radioactive Molecules"
— Kieran Flanagan (University of Manchester), "Table top nuclear facility for molecular spectroscopy"
— Tim Langen (TU Wien), "Searches for symmetry violations with laser-cooled BaF molecules"
— Stephan Malbrunot-Ettenauer (University of Toronto), "Exploring new physics beyond the standard model of particle physics using radioactive molecules at TRIUMF"
— Victoria Vedia (CERN) TBA
— Yan Zhou (University of Nevada, Las Vegas), "Toward a measurement of nuclear Magnetic Quadrupole Moment using quantum logically controlled molecular ions"

Theory

— Antoine Belley (MIT), "Parity Violating In Medium Similarity Renormalization Group"
— Anastasia Borschevsky (University of Groningen), "Testing the Standard Model with molecules : theoretical perspective"
— Evgeny Epelbaum (Ruhr University Bochum), "Parity- and Time-Reversal-Violating Nuclear Forces"
— Christian Forssén (Chalmers), "Uncertainty quantification of nuclear forces"
— Matthias Heinz (Oak Ridge), "First-principles nuclear structure theory and implications for fundamental physics"
— Jason Holt (TRIUMF), "First-principles nuclear theory for new physics searches"
— Petr Navrátil (TRIUMF), "Ab initio calculations of electric dipole, Schiff, and anapole moments in atomic nuclei"
— Herlik Wibowo, (University of York), "Calculation of nuclear Schiff moments from DFT"

IV. PRELIMINARY PROGRAM

We plan to have three one-hour talks per day, with ample time for discussion, plus some dedicated discussion sessions.

Day 1	Day 2	Day 3	Day 4	Day 5
10h00 Epelbaum	10h00 Langen	10h00 Forssén	09h30 Holt	10h00 Zhou
11h00 **Break**	11h00 **Break**	11h00 **Break**	10h30 **Break**	11h00 **Break**
11h30 Flanagan	11h30 Navrátil	11h30 Garcia Ruiz	11h00 Delahaye	11h30 Wibowo
12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**	12h30 **Lunch**
14h00 Borschevsky	14h00 Malbrunot-Ettenauer	14h00 Belley	14h00 Heinz	14h00 Vedia
15h00 **Break**	15h00 **Break**	15h00 **Break**	15h00 **Break**	15h00 **Break**
15h30 Discussions	15h30 Discussions	15h30 Discussions	15h30 Discussions	15h30 Discussions
17h00 End	17h00 End	17h00 End	17h00 End	17h00 End

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