Beta decay gets the ab initio treatment

Beta decay is one of the fundamental radioactive decay modes of nuclei. Now, for the first time, nuclear theorists have been able to explain nuclear beta decay properties across a range of isotopes up to atomic mass 100 from a wide set of first-principles simulations.

The theoretical modelling of nuclei and their different decay modes is a challenging field. Take β decay, for instance, which affects the vast majority of radioactive isotopes. For years, the most accurate theoretical calculations of nuclear structure, which agreed with experiments on masses and shell structure, predicted Gamow-Teller β-decay half-lifes that were off compared to experiments. Practitioners had to quench their calculations by about 25 % to reproduce experimental values. The origin of this "quenching puzzle" remained elusive for decades. Now, in a paper by Gysbers *et al.*, a collective of theorists based in the US and Canada has, for the first time, provided a solution to this puzzle based on first-principles simulations.

In the past decade, the so-called *ab initio* revolution has changed the way that nuclear theory and, more generally, nuclear physics operates on a daily basis. New nuclear interactions, derived from the theory of quantum chromodynamics, and advances in computational resources have allowed for a truly first-principles description of nuclear structure[1]. Compared to the more traditional phenomenological or density functional calculations, *ab initio* simulations allow for a consistent treatment of systematic errors and offer a significantly different level of predictive power, as they have virtually no parameters and are directly informed by the underlying theory of the strong force.

Most early *ab initio* calculations were used to study nuclear masses. Over time, however, the reach of these calculations was extended substantially, from closed to open-shell isotopes, and from masses to nuclear radii[2], electromagnetic observables[3] and even nuclear reactions[4]. At present, the most stringent limitation of these methods is computational power, which limits the number of particles that can be simulated. Currently, *ab initio* calculations can reliably predict properties for isotopes up to mass number $A \approx 100$.

The study of radioactive decays was conspicuously missing in the recent wave of *ab initio* predictions. β decay is the most common of such radioactive decay modes, and operates in two possible ways. In β- decays, a mother isotope of Z protons and N neutron decays into a daughter isotope of Z+1 protons and N-1 neutrons, while emitting an electron and an anti-neutrino. β+ (or positron) decays operate in a similar fashion, but the daughter nucleus has Z-1 protons and N+1 neutrons, accompanied by the emission of a positron and a neutrino. Further, the spin alignment between the positron (electron) and the (anti)neutrino determines whether the decay is a Fermi (anti-parallel alignment) or a Gamow-Teller (parallel) decay.

The theoretical description of Gamow-Teller β decays is a notoriously difficult problem. In theoretical terms, the half-lifes of these decays is inversely proportional to a quantity called the Gamow-Teller matrix element. An accurate calculation of these matrix elements requires knowledge of at least two different physics aspects. On the one hand, one needs a relatively accurate description of the nuclear shell structure of both the mother and daughter nucleus. On the other, one requires an understanding of how the weak interaction operates within a many-body environment like the interior of a nucleus. The latter is contrast to the weak decay of a single neutron, which is a well understood problem since Fermi's pioneering work[5].

Unfortunately, for a long time, nuclear theorists could not perform a consistent calculations of both nuclear ground states and the renormalization of the weak interaction in a nucleus. While there were indications that this renormalization was important, a full understanding of the “quenching puzzle” required at least three ingredients that precluded a full solution for decades.

First, the puzzle couldn’t be resolved by looking at the decay of a single isotope. Shell structure can affect Gamow-Teller matrix elements in very different ways, and the puzzle in fact affects many different nuclei. Figure 1 shows all the 28 isotopes that have been studied in this work. Key among them is the extraordinary isotope ^{100}Sn, the heaviest known doubly-closed-shell nucleus with *N=Z=50*, and the isotope with the strongest observed Gamow-Teller strength. Simulations of this isotope are a *tour de force* for *ab initio* methods, at the limit of what is computationally possible. Perhaps more importantly, the production of this isotope has been and remains an experimental challenge on its own[6].

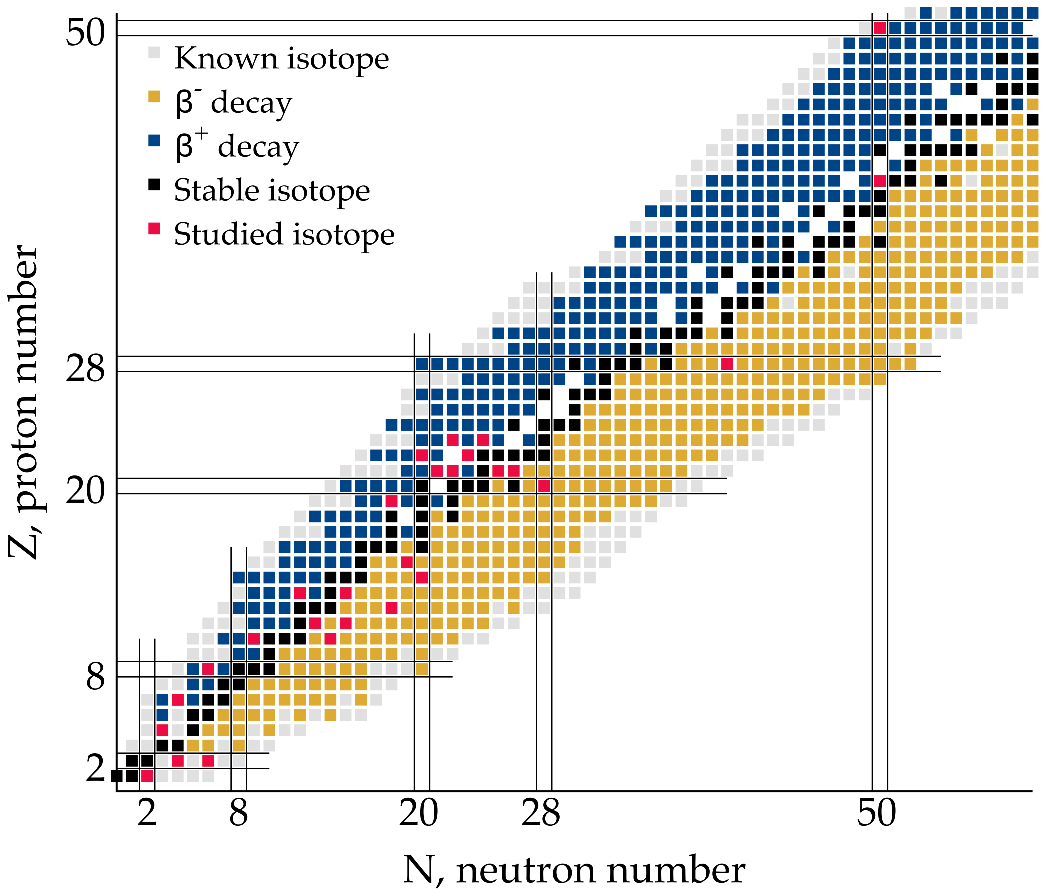

Figure 1: Section of the Segrè chart for elements between hydrogen (Z=1, bottom) and tin (Z=50, top) [7]*. In this region, most isotopes decay predominantly by β decay, either by emitting an electron (β- decay, yellow squares) or a positron (β+ decay, blue squares). Gisbers et al. have studied the isotopes marked in red, and have found a remarkable level of agreement with experimental data.*

Second, a convincing resolution required not only one, but several *ab initio* schemes. There are different first-principles methods to solve the quantum many-body problem, and each introduces its own type of approximation. Gisbers *et al.* use three different approaches. In fact, one of them (the coupled cluster method) has been extended to treat Gamow-Teller transitions for the first time, which is in itself an impressive technical feat. Importantly, all these different methods are benchmarked in different nuclei to quantify uncertainties, which remain at the level of 10%. Solving the puzzle with these three methods allows for an unambiguous identification of the role of many-body correlations.

Third, these *ab initio* calculations needed to start from the same (and consistent) strong and weak interaction Hamiltonians. Here, chiral effective field theory has been the key tool to establish consistency between the two. Using different chiral hamiltonian ensures that any systematics from unknowns in the strong and the weak interaction are propagated into the Gamow-Teller matrix elements.

With these three breakthroughs, Gisber *et al.* are able to reproduce experimental data on Gamow-Teller matrix elements on isotopes as light as helium and as heavy as tin from first principles. By implementing different numerical tests, they conclude that a microscopic explanation of the puzzle requires both many-body correlations in the nuclear wavefunctions and corrections to the weak interaction in the medium. In ^{100}Sn, these corrections are of similar sizes and both are necessary to reproduce experimental results.

This is the first of future incursions of *ab initio* theory into the realm of nuclear decays. At the level of Gamow-Teller decays, one can expect a series of improvements and better agreement with data, as *ab initio* calculations become more accurate. β decay is also at the basis of key astrophysical processes, like the rapid neutron capture process, responsible for the production of over 50% of elements above iron. Current simulations of these processes require Gamow-Teller matrix elements in isotopes that have not been studied experimentally. *Ab initio* calculations now have the potential to tackle some of these experimentally unknown decays from first principles, which will no doubt inform astrophysical simulations on a firmer basis.

More importantly, the lessons learned in understanding β decay pave the way forward for other relevant radioactive decay modes. If the neutrino is its own antiparticle, for instance, an extremely rare nuclear decay called neutrinoless double-β decay should be possible. A number of experiments have been designed to detect this elusive decay mode. A key uncertainty in these experiments is the so-called nuclear matrix element, which plays a role akin to the Gamow-Teller matrix elements of standard β decay. *Ab initio* calculations can now address the isotopes involved in these experiments, and thus could provide a much-needed first-principles footing on neutrinoless double-β decays in the near future.

1. Hagen, G. *et al.* Neutron and weak-charge distributions of the 48Ca nucleus. *Nat Phys* **12,** 186–190 (2016).
2. Lapoux, V. *et al.* Radii and Binding Energies in Oxygen Isotopes: A Challenge for Nuclear Forces. *Phys. Rev. Lett.* **117,** 052501 (2016).
3. Parzuchowski, N. M., Stroberg, S. R., Navrátil, P., Hergert, H. & Bogner, S. K. Ab initio electromagnetic observables with the in-medium similarity renormalization group. *Phys. Rev. C* **96,** 1–17 (2017).
4. Hupin, G., Quaglioni, S. & Navrátil, P. Ab initio predictions for polarized deuterium-tritium thermonuclear fusion. *Nat. Commun.* **10,** 351 (2019).
5. Fermi, E. Versuch einer Theorie der β-Strahlen. I. *Zeitschrift für Phys.* **88,** 161–177 (1934).
6. Hinke, C. B. *et al.* Superallowed Gamow–Teller decay of the doubly magic nucleus 100Sn. *Nature* **486,** 341–345 (2012).
7. Audi, G., Kondev, F. G., Wang, M., Huang, W. J. & Naimi, S. The NUBASE2016 evaluation of nuclear properties. *Chinese Phys. C* **41,** 1–138 (2017).