Excerpt from DBD Topical Collaboration Final Report

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2 Goals

At the start of our grant period, the hadronic and nuclear matrix elements that allow the extraction of fundamental physics from the rate of neutrinoless double-beta ($0\nu\beta\beta$) decay and the magnitude of electric dipole moments were quite uncertain. The uncertainty in the matrix elements for $0\nu\beta\beta$ decay was typically taken to be about a factor of three but that number, which came simply from comparing the predictions of apparently reasonable models, was an underestimate; it ignored the possibility that all models had missed significant physics.

As noted in prior-year reports, the goals of our collaboration were more accurate calculations of these matrix elements, with quantified uncertainties. Reaching the goals was a major challenge. To overcome it, our collaboration proposed a careful path forward, starting with attempts to understand physics that affects double-beta decay in the nuclei used in experiments and also manifests itself in light nuclei, which can be more easily treated theoretically. An important intermediate goal was an account of the crucial quenching of g_A. We reached that goal in years 3 and 4. After that we began the *ab initio* computation of double-β matrix elements, culminating with calculations in ^{48}Ca by two separate groups, and the beginning of a computation in ^{76}Ge. This report details these and other achievements, while also noting what still remains to be done.

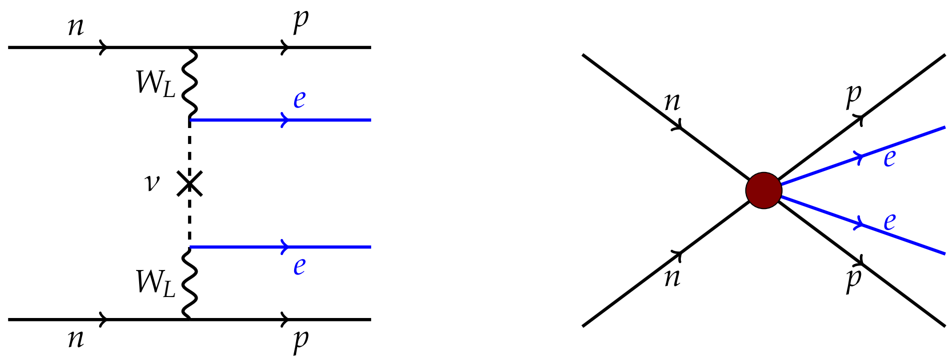

Figure 1: The leading diagrams in χEFT for $0\nu\beta\beta$ decay induced by the exchange of a light Majorana neutrino. The first diagram contains the explicit exchange of a low-energy neutrino, and the second a short-range counter term coming from a virtual neutrinos with energy above about 1 GeV.

3 Accomplishments

3.1 Double-Beta Decay

(A) Introduction

The occurrence of $0\nu\beta\beta$ decay would mean that neutrinos are Majorana particles (their own antiparticles) and that some new lepton-number-violating physics is responsible [1]. The importance of the decay has led experimental groups all over the world to try to observe it. The experiments are difficult and expensive, however, and good decisions about how much and what kind of decaying material to use are crucial. The rate of the decay depends on nuclear matrix elements that are calculable but impossible to measure, and so experimentalists require reliable calculations to to inform their choices. At the beginning of our collaboration, the theory needed to compute the matrix elements carried an uncertainty that couldn't even be estimated convincingly [2].

Over the five years of DOE funding, we made great progress in the computation of the $0\nu\beta\beta$ matrix elements. Doing so necessitated a better understanding of physics at several scales: a TeV or above, where interactions among new particles responsible for $0\nu\beta\beta$ decay occur, in the region between a TeV and a GeV, where QCD affects decay rates in unexpected ways, and at a few MeV, where the nuclear many-body problem is the main issue. In addition to working on this last problem, previously thought to be the whole story, the collaboration began to address the important questions in QCD, and also developed a chain of effective theories that specify how the physics at one scale is summarized in the couplings and masses of the effective theory that describes lower-energy processes at the next.

We discuss each of these programs and how they link together.

(B) EFT

Chiral EFT: Over the last 20 or so years, theorists have made a concerted effort to use a chiral effective field theory (χEFT) of pions and nucleons, with higher-mass particles and higher-energy physics "integrated out," to describe and predict features of nuclear structure. The effort includes the systematic treatment of weak currents, which are obviously important for $0\nu\beta\beta$ decay. But because the virtual intermediate neutrino in that process can have an arbitrarily high energy, the decay is caused by more than just the combined action of two low-energy weak currents That means that the $0\nu\beta\beta$ operator, even for light neutrino exchange and even forgetting about many-body contributions to the weak current, contains more than the usual simple diagram on the left of Fig. 1 if degrees of freedom beyond nucleons and pions are integrated out of the description.

In a series of papers over the last few years, our groups at Los Alamos (LANL) and Berkeley (UCB), with their collaborators, formulated the correct extension of χEFT to $\beta\beta$ decay. Ref. [3], building on earlier work by Prézeau, Ramsey-Musolf, and Vogel [4], lays out that theory for heavy particle exchange, which might contribute as much to the rate of $0\nu\beta\beta$ decay as light-neutrino exchange, and shows how the parameters that determine the rates of very heavy-particle lepton-number violating physics work their way down into the nucleon level-double beta decay operator. They supplemented that work with a more systematic treatment [5, 6], obtaining a "master formula" that describes the $0\nu\beta\beta$ decay rate as a specific combination of of phase-space factors, nuclear matrix elements, hadronic low-energy constants, QCD evolution factors, and high-energy lepton-number-violating Wilson coefficients. The master formula can be easily matched to any model where lepton-number violation originates above the electroweak scale

The group's Ref. [7] is a preliminary examination of light-neutrino exchange, showing that at the 10% level of accuracy one must consider many "non-factorizable" diagrams (those that cannot be broken in two by cutting the line representing the exchanged neutrino) that had heretofore been neglected. In Ref. [8] the LANL Quantum Monte Carlo (QMC) group evaluated the matrix elements of the new diagrams in light nuclei, where *ab initio* wave functions are available. In Refs. [9, 10, 11, 12, 13, 14] the Central Michigan (CMU) group examined the same contributions, though in an older formulation of them, in the shell model.

Shortly after publishing their χEFT formulation, the LANL group made the additional startling discovery [15] that a contact diagram, representing the effects of high virtual-neutrino momenta that are integrated out of the pion-nucleon effective theory, occurs at the same order in chiral perturbation theory as the usual lower-energy neutrino exchange diagram, i.e. at leading order. This contact diagram, shown on the right of Fig. 1 had never been considered before. In Ref. [16], the group confirmed the finding in a number of regularization schemes and showed that no other unknown coefficients appear at next-to-leading order. In the same paper they explored the connection between $0\nu\beta\beta$ decay and nuclear charge-independence breaking induced by electromagnetism. From *ab initio* quantum Monte-Carlo calculations for ^{6}He and ^{12}Be, they concluded that, at least in light nuclei, the leading short-range operator has a sizable impact on the $0\nu\beta\beta$ matrix elements.

Just before the end of the topical collaboration, the LANL group was able to estimate the coefficient of the contact term [17, 18]. Their approach was based on the representation of the amplitude as the momentum integral of a known kernel (proportional to the neutrino propagator) times the generalized forward Compton scattering amplitude $n(p_1)n(p_2)W^+(k) \to p(p_1')p(p_2')W^-(k)$, in analogy with the Cottingham formula for the electromagnetic contribution to hadron masses. They constructed model-independent representations of the integrand in the low-momentum region with chiral EFT and in the high-momentum region with the operator product expansion, and then constructed a model for the full amplitude by interpolating between the two regions, using nucleon form factors for the weak currents and information on nucleon–nucleon (NN) scattering in the $^1S_0$ channel away from threshold. By matching the amplitude obtained in this way to the leading-order chiral EFT amplitude, they obtained the relevant leading-order contact term with a quantified uncertainty. They expressed the final result as a scheme-independent renormalized amplitude at a set of kinematic points near threshold. Any practitioners, using their own renormalization schemes, can determine the coefficient of the contact term by adjusting it to reproduce this amplitude. One of our many-body groups has already done so, as we will discuss later.

The LANL group also examined the potential role of sterile neutrinos in $0\nu\beta\beta$ decay. They worked with collaborators in a model-independent extension of the standard model to parameterize $0\nu\beta\beta$ rates in terms only of neutrino masses and known quantities (or calculable ones, such as nuclear matrix elements) [19]. The results should prove useful in global analyses of sterile-neutrino searches. The group found that non-standard interactions involving sterile neutrinos have a dramatic impact on $0\nu\beta\beta$ phenomenology, and next-generation experiments can probe such particles up to scales of $\mathcal{O}(100)$ TeV.

HOBET: The Berkeley group focused on an alternative approach, Harmonic Oscillator Basis Effective Theory (HOBET). Though it has not yet been applied to $\beta\beta$ decay, the theory, based on a separation of short- and pion-range physics that is more realistic than in χEFT and avoids the intermediate step of a soft potential, is very promising. During the time of the collaboration the Berkeley group developed an efficient procedure for fixing the low-energy constants (LECs) directly from phase shifts [20] and worked out in detail the separation between short and long-range physics [21]. The paper in which the separation was accomplished is a review that also included a discussion of HOBET's interface with lattice QCD and included members of our lattice group as authors (see next section). The ease with which rectangular and spherical bases can be interchanged in the harmonic oscillator makes allows HOBET be embedded in a finite box leading to a nice alternative to Lüscher's method for infinite-volume extrapolations.

Although the method has only been applied to systems of two and three nucleons so far, it promises to be useful in many-body calculations of $\beta\beta$ matrix elements. An initial paper on the many-body version of the theory will appear soon.

(C) Lattice QCD

Our lattice QCD group will eventually be able to determine the contact coefficient discussed in the previous section with better precision than the model-dependent analysis. But during the collaboration period it already provided coefficients of some of the other operators in the $\beta\beta$ EFT. Figure 2 below shows one of the leading contributions to $0\nu\beta\beta$ decay produce by the exchange of beyond-Standard-Model (BSM) heavy particles (inside the red blob). The exchange occurs between two pions, which makes it easier to handle than the direct exchange between nucleons. The lattice group, together with their collaborators, determined the dependence of the coefficient representing the red blob on the four-quark operators that the BSM physics specifies [22]. Their work includes a diffi-

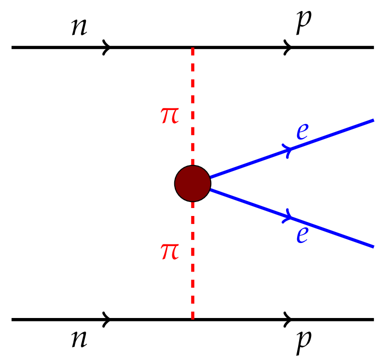

Figure 2: The leading contribution to $0\nu\beta\beta$ decay that is mediated by heavy-particle exchange. The TC lattice group has determined the dependence of the coupling represented by the red blob on the underlying model of lepton-number violation.

cult non-perturbative operator renormalization [23] that will pay dividends when other processes involving two- or three-nucleon states are addressed.

Within the two-nucleon sector, the methods must be generalized to allow the analysis of the diagrams in which nucleons couple directly to the heavy particles. Before these may be faithfully calculated, the group must produce good two-nucleon operators. In the meantime, the group and collaborators have begun tests in lattice chiral-EFT for extracting the appropriate couplings from full QCD calculations [24] (the optimal versions of which are still to be carried out).

The group has of course been exploring several methods for obtaining the good two-nucleon operators just mentioned. Using Matrix Prony, a method similar to variational methods in which linear combinations of multiple different operators are determined to maximize overlap onto the desired states, the group has computed nucleon-nucleon scattering observables with an artificial pion mass of only 350 MeV, the lowest attempted to date [25]. Using a method called sLapH [26], developed to scale more favorably with the volume than other variational methods, they obtained results [27] that were in stark disagreement with those from other lattice collaborations that used local hexaquark operators. Preliminary research into the disagreement is leading to a community-wide reassessment of multi-nucleon processes on the lattice.

The group has also investigated ways in which to treat the usual light-neutrino exchange represented at the nucleon level by the diagrams in Fig. 1. One avenue is the use of massive neutrino propagators in order to avert some of the issues associated with massless fields in a finite volume. In collaboration with other researchers, our group studied a similar formalism: the use of massive photons for studying QED effects on hadronic physics. The first publication, which identifies a suitable parameter space for controlling systematics in such a formalism, is forthcoming.

Finally, the lattice group published a precision calculation of g_A (the "bare" value rather than the quenched one we discuss next). A result with percent-level accuracy [28, 29] appeared in the journal *Nature* [30]. They followed this project up with work on the nucleon axial form factor, at momentum transfers up to about 2 GeV. In the process, they improved their result for g_A to the 0.5% level [31, 32].

Our lattice work led to several joint reviews by our LANL, UCB, and UNC groups (plus collaborators), including one on ways to connect the physics of rare nuclear processes to the underlying quark- and gluon-level operators [33] and another on grounding nuclear physics in QCD [21]. The UNC group also was part of the lattice community's official cross-group averaging process [34].

(D) Learning from Light Nuclei and Tests

Any $\beta\beta$ decay occurring in light nuclei would be swamped by successive single-β decays, and so no such nuclei are used in experiments. One may still compute the matrix elements for their decay, however, to explore ideas and test methods in systems that allow nearly exact solutions to the Schrödinger equation.

As we've noted, Our collaboration focused on the use of *ab initio* methods with controlled uncertainty. In this section we describe the wide range of computations in light systems that we undertook in preparation for an attack on the heavier systems of interest to experimentalists.

Softening of Operators: An important step for many *ab initio* methods, including several we adopted, is a unitary transformation that decouples high- and low-momentum components of the nuclear interaction, producing "soft" operator for use at low momentum and easing calculations in large model spaces. Our group at Livermore used the similarity renormalization group (SRG) to obtain the transformation. In an A-nucleon system, the beneficial decoupling of momentum scales comes at the price of an effective Hamiltonian containing irreducible three- and higher-body (up to A-body) terms, even when such terms are not present in the initial (bare) Hamiltonian. And the same unitary transformation must be applied to the $0\nu\beta\beta$ operator, again inducing many-body pieces.

The LLNL group first applied these ideas to single-β decay, computing one- and two-body corrections to the bare one-body operator and contributing to important work explaining the longstanding "g_A quenching puzzle" (which we describe in detail shortly). They then turned to $0\nu\beta\beta$ decay, computing two- and three-body corrections to the bare two-body transition operator for light-neutrino exchange. The effects of the renormalization were then tested through no-core shell model (NCSM) and valence-space in-medium SRG (VS-IMSRG) calculations of the $0\nu\beta\beta$ matrix elements for the decay of selected even-even nuclei: ^{6}He, ^{8}He, ^{10}Be, ^{10}He, ^{14}C and ^{48}Ca (Fig. 3). The three-body induced terms turn out to be important, but except for the Gamow-Teller matrix element in ^{10}He, the variation of matrix elements with the SRG resolution scale λ decreases as two- and three-body corrections are successively included, a good result. A manuscript detailing these results is currently in preparation [35].

Exploring Generic Features of Weak Transitions: We have already mentioned briefly the work of the LANL group and collaborators that used QMC to investigate the chiral expansion of $0\nu\beta\beta$ operators in light nuclei. The group also compared shell-model and variational Monte-Carlo calculations of $0\nu\beta\beta$ decay in the $A = 10$ and $A = 12$ systems [36], finding some differences but mostly similarities in the two approaches. Finally, they used quantum Monte Carlo to compute single-β-decay rates in sd-shell nuclei, with interactions

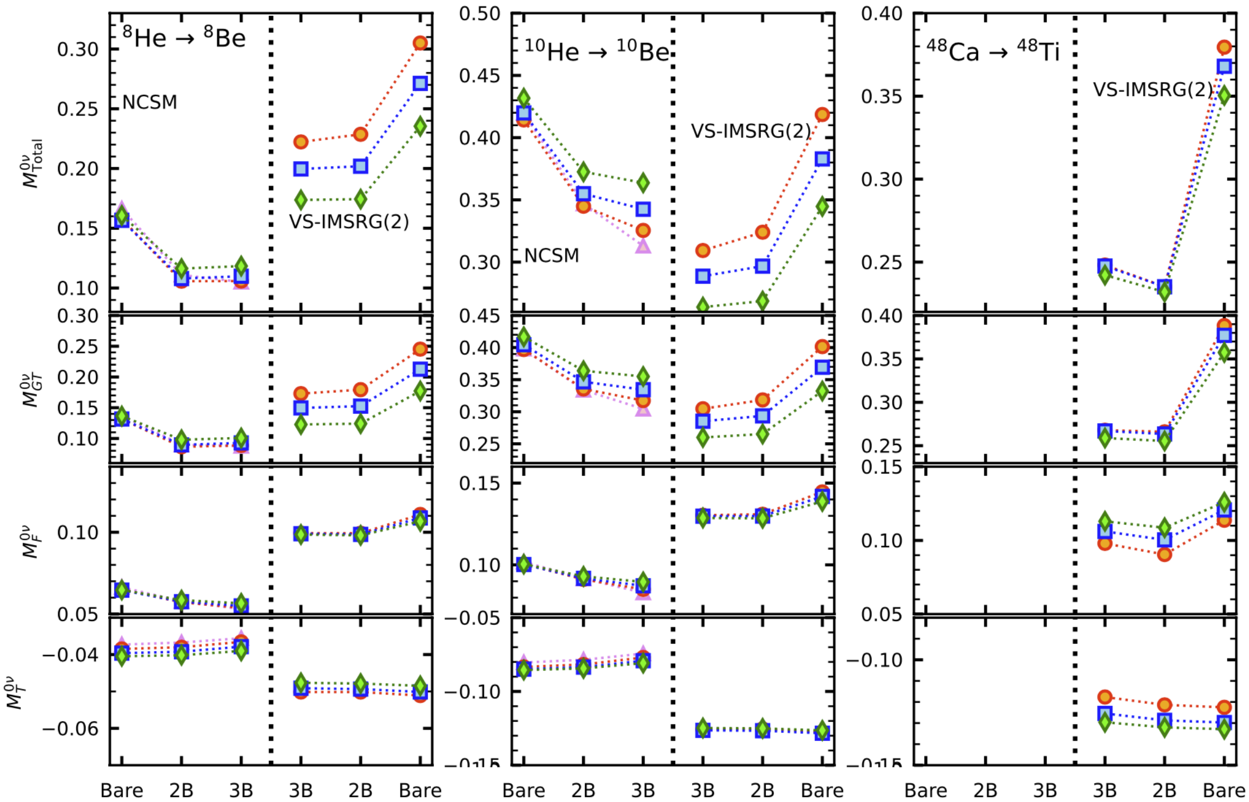

Figure 3: SRG corrections to nuclear matrix elements in light and medium nuclei, for several resolution scales (colors) and two many-body methods, the quasi-exact No Core Shell Model (NCSM), and the valence-space in-medium similarity renormalization group (VS-IMSRG(2)).

and currents from chiral EFT [37]. The roles of correlations in the nuclear wave functions and of two-body currents, while small in very light nuclei, grow considerably by $A = 15$. This work ties to the explanation of g_A quenching that we will discuss shortly.

Tests of *Ab Initio* Methods: *Ab initio* many-body methods start with interactions and operators determined from QCD and/or fit to data in very light nuclei ($A = 2, 3,$ or 4), and then solve the Schrödinger equation, approximately, in heavier nuclei. Our collaboration was able to employ two distinct *ab initio* methods in the heavy open-shell nuclei of interest to experimentalists:

- *In-Medium Generator-Coordinate Method (IM-GCM)*: The in-medium SRG, developed over the past 15 or so years [38], adapts the similarity renormalization group discussed above so that it decouples low-lying nuclear states nuclei from high-lying ones rather than high- and low-momentum two- and three-particle states. It requires a reasonable approximation to the ground state of the nucleus of interest to construct (and then solve) the renormalization-group equations. In closed shell nuclei, a Slater determinant will suffice as an approximation but in more complicated nuclei we need a state that takes into account collective degrees of freedom such as deformation and pairing. To construct it, the MSU and UNC groups [39] developed a variation that uses the generator coordinate method (GCM), which superposes symmetry-violating mean field states with a range of deformations, pairing gaps, etc., and projects out pieces of each that conserve angular momentum and particle number. The resulting approximate ground state contains the important collective correlations, allowing the renormalization-group equation to incorporate the physics that it treats best — non-collective excitations — into an effective interaction and $\beta\beta$ decay operator.

- *Coupled-Clusters Theory*: The coupled-clusters approach starts with an exponential ansatz for the ground state of an even-even nucleus: $|\Phi\rangle = e^{A}\,|HF\rangle$, where $|HF\rangle$ is the Hartree-Fock Slater determinant and A contains operators that create particles and holes. Even if one truncates A to include only few-particle few-hole excitations, one gets a good approximation to the ground state because the exponentiated operator creates many-particle many-hole excitations. To apply the approach to $\beta\beta$ decay, one needs to represent the ground state of one of the two nuclei in the decay as a two-proton two-neutron-hole (or vice versa) excitation of the other, with additional neutron-neutron and proton-proton particle-hole corrections. A version of the formalism that allows deformed states is necessary for most nuclei. The UT group developed both the deformed version of the procedure and thee ability to include proton-particle neutron-hole excitations. They also created a version of coupled-clusters theory that leads to an *ab initio* valence-space shell-model effective interaction [40].

Our collaboration made extensive the use of light nuclei to test the accuracy of the many-body methods that are designed for heavy nuclei by comparing their results with those of more accurate methods — Quantum Monte Carlo and the No-Core Shell Model — that are restricted by computational issues to light nuclei. We also wanted to compare the heavy-nucleus methods with one another. In addition to assessing the viability of our methods, this benchmarking allowed us to identify coding errors. Benchmarking projects included the following:

- The MSU, ISU, and UNC groups combined for a benchmark of the No-Core Shell Model (NCSM) and the IM-GCM, used, as we'll see later, for calcuations in ^{48}Ca and ^{76}Ge) for the artificial $0\nu\beta\beta$ decay of ^{6}He [41]. Although there were some differences in the ground-state energies predicted by the two methods, the matrix elements of the $0\nu\beta\beta$ operator are remarkably close in the two approaches. Neither result changes significantly with the addition of more shells.

- The UT and LLNL groups use *ab initio* NCSM calculations for transitions in light nuclei to gauge the quality of coupled-cluster computations of $0\nu\beta\beta$ decay [42]. We'll describe the successful use of coupled-clusters techniques to compute the decay matrix element of ^{48}Ca later.

- The MSU group and collaborators benchmarked both the IM-GCM and a valence-space variant against the NCSM and coupled cluster result in nuclei up to $A = 22$ [43]. The matrix elements did not always agree perfectly, but were consistent with one another.

- The LLNL and MSU groups both completed the ordinary-SRG evolution (mentioned above) of $\beta\beta$ operators at the two-body level, with LLNL working in an oscillator basis and MSU in a plane-wave basis. At the highest energies there are slight discrepancies, but at low energies the agreement is essentially perfect.

- The ISU group validated the Lee-Suzuki-Okuba formalism that underlies the NCSM in an artificial system consisting of two neutrons in a trap [44].

- The UT, MSU, and UNC groups, with additional collaborators, carried out a similar benchmark between the coupled-cluster equation of motion method, the IM-GCM, and the NCSM in a range of light isotopes. The agreement among the three methods is promisingly good.

- The UNC and CMU groups, plus collaborators, tested the GCM (without any SRG) a valence space against full shell-model calcuations in Refs. [45, 46]. Though the nuclei in which tests were conducted (^{76}Ge, ^{124}Sn, ^{130}Te, ^{136}Xe) were not light, the agreement was nonetheless good. The GCM underlies the IM-GCM mentioned in the first benchmark.

  In related work, the SDSU group investigated a way to make the GCM more efficient by choosing the mean-field states that make up the computations basis in a more sophisticated way. The promising results [47] will eventually improve the IM-GCM.

- Finally, as we've already hinted, the MSU group evaluated the change in nuclear matrix elements caused by the χEFT contact term discussed in section (B) [48]. The contact term increases the matrix elements in all cases investigated so far (^{6}He, ^{8}He, and ^{48}Ca).

(E) Quenching of g_A and Connection with $0\nu\beta\beta$ Decay

We cannot hope to understand $\beta\beta$ decay without understanding single-β decay, which has challenged us for many years. Both single-β and two-neutrino $\beta\beta$ decay rates have both been over-predicted by phenomenological nuclear structure calculations, and getting correct rates has required the *ad hoc* use of a reduced value for the axial vector coupling constant g_A. Fortunately, the "quenching" factor is nearly constant for nuclei in the same mass region and varies slowly as mass is increased. Still, unless we understand the source of the quenching we do not know whether $0\nu\beta\beta$ rates are also being over-predicted, and by how much if they are.

From the EFT point of view, the quenching can be due only to deficiencies in many-body models (and for the shell model that means truncation of the full A-particle Hilbert space) and/or many-nucleon currents arising from pion exchange and higher-energy physics. Our collaboration has investigated both sources. In Ref. [37], as we noted earlier, the Los Alamos group carried out QMC calculations of β decay in a range of light nuclei with mass-number A between 6 and 10. They were able to examine the effects of both correlations and two-nucleon currents on the corresponding matrix elements and found that the former can cause a 10% reduction while the effects of the latter are at the $2-3\%$ level, and sometimes actually increase the matrix elements rather than quenching them.

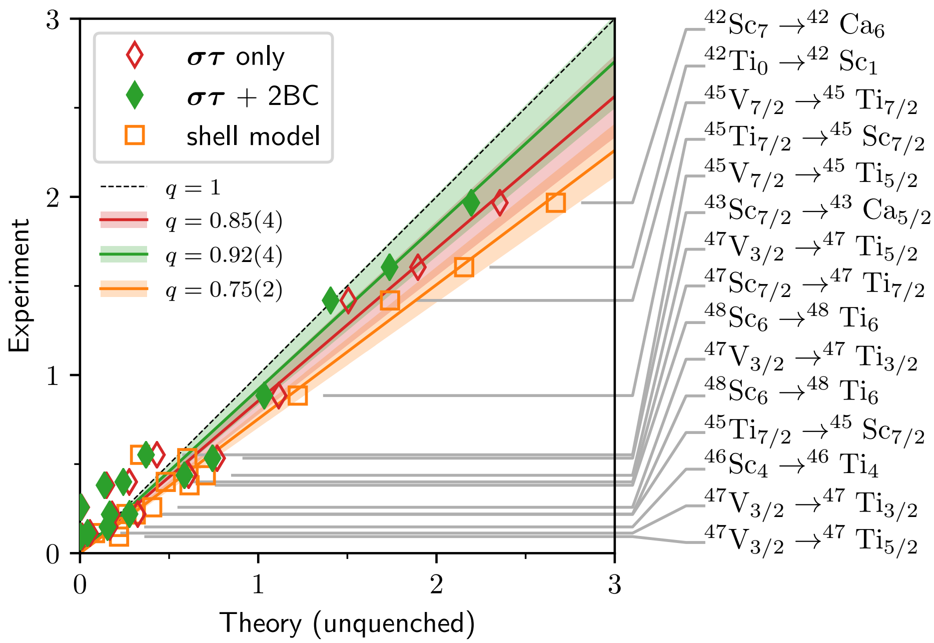

Figure 4: From Ref. [49], experimental GT matrix elements vs. calculated versions for a number of β transitions. The squares represent results of from the phenomenological shell model, the open diamonds results of the shell model with renormalized interactions and decay operators, and the solid diamonds the results when two-body currents are added alongside the renormalized operators. The dotted line with slope 1 indicates perfect agreement between theory and experiment.

These conclusions, while valuable because of the reliability of QMC, are hard to extrapolate to much heavier nuclei. But other *ab initio* many-body methods, including coupled-clusters theory and the VS-IMSRG were able to treat those nuclei. Our groups at ORNL and LLNL, together with a TRIUMF-INT group, computed β-decay rates in a whole range of nuclei, from the sd shell up to ^{100}Sn. They found that comprehensive many-body correlations and two-body currents produce quenching that is large and nearly reproduces experiment. Figure 4 illustrates this result. Once both correlations from outside the valence shell and two-body currents are included, g_A needs to artificially quenched only by a factor of 0.92 (rather than the factor of 0.75 one needs without those ingredients). And, unlike in much lighter nuclei, the effects of two-body currents are always significant. It is actually not surprising that those effects are larger in heavier nuclei than in very light ones because the contribution of each "spectator" nucleon (the nucleon in the two-body-current-pair that doesn't change from neutron to proton) combines coherently with the others. NCSM calculations by the LLNL group and collaborators verify both the modest quenching of two-body currents in light-nucleus QMC calculations and the more significant quenching in the some of the (slightly) heavier-nucleus coupled-cluster and VS-IMSRG calculations. The results, which appeared in *Nature Physics* [49], convincingly show that both correlations and two-body currents are required to account for the full quenching. The quenching problem has thus been mostly solved.

The same two-body currents that quench β decay will also have an effect on $0\nu\beta\beta$ decay. χEFT suggests that their effects are not large, but the importance of the g_A question (and the fact that the $\beta\beta$ matrix elements contain two powers of g_A) demands a more

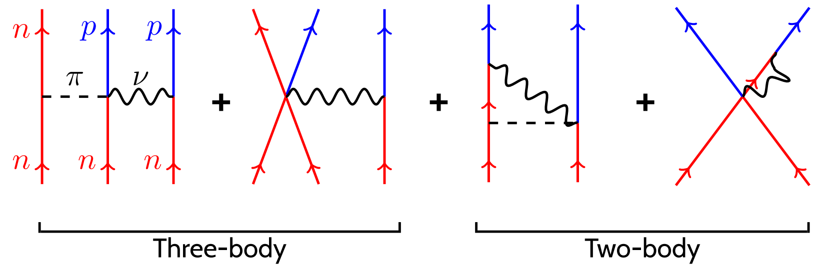

Figure 5: Diagrams representing three-body and two-body effective $0\nu\beta\beta$ operator produced by the action of one one-body current and one two-body current. Electron lines are omitted.

careful investigation. The UNC, MSU, and SDSU groups examined [50] the effects of two-body weak currents with shell-model wave functions. The two-body currents generate three-body double-beta operators. When they folded their three-body matrix elements with the shell-model wave functions, the groups found the quenching to be not only less than that affecting single-β decay but also less than initial studies of $\beta\beta$ decay indicated [51]. The authors also looked at *two-body* double-beta operators that are generated by the two-body weak currents, from loop diagrams, finding their effects to be moderately small as well when evaluated in a traditional way. (Figure 5 depicts the two- and three-body operators.) Within a completely consistent χEFT treatment, however, one should add to one's calculation a previously overlooked contact two-body double-beta operator, the strength of which is unknown. This is the same issue as that found at leading order by our LANL group (and later resolved for the that case, as we've discussed in the EFT section).

(F) *Ab initio* $0\nu\beta\beta$ Elements in Nuclei Used in Experiment

^{48}**Ca** : Much of our focus was on ^{48}Ca, the lightest nucleus whose $\beta\beta$ decay is not swamped by successive single-β decays, and therefore the lightest of interest to experimentalists [52]. Because it is relatively light and doubly magic, it is also the easiest for us to address with *ab initio* many-body techniques.

Using the newly developed IM-GCM (see Sec. (D)), the MSU and UNC groups were the first to complete a calculation of the light-neutrino-exchange $0\nu\beta\beta$ matrix element in this nucleus [53]. Their initial paper included just the leading order long-range piece (Sec. (B)). The correlations included by the *ab initio* approach, responsible for most of the g_A quenching with an effect on $0\nu\beta\beta$ decay, resulted in a matrix element that was smaller that those from phenomenological models (see Fig. 6; the IM-GCM matrix element is labeled IMSRG+GCM). A second paper by the MSU group [48], already mentioned, used the procedure spelled out in Ref. [17] to include the effects of the newly discovered contact term. The additional piece increased the matrix element by about 40%, bringing it close to earlier shell-model predictions. These results together suggest that the large quenching feared by some is unlikely.

The initial IM-GCM work was followed shortly after by a paper [42] from the UT, LLNL, and UNC groups (plus collaborators) that applied the coupled-clusters methods described above to the same ^{48}Ca decay. This paper was the first application of deformed-basis coupled-clusters theory. The full results, without the contact term (which wasn't yet

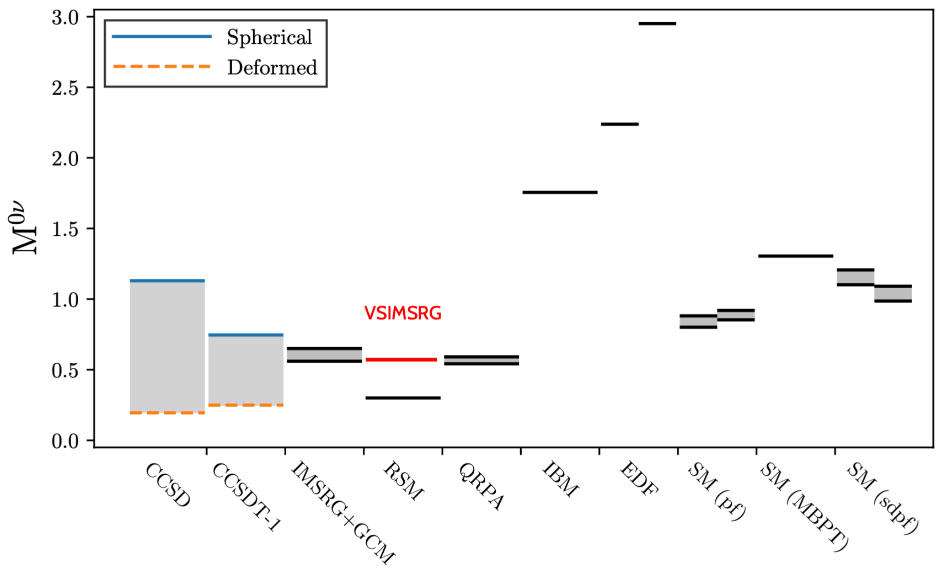

Figure 6: Comparison of the nuclear matrix elements for the decay of ^{48}Ca predicted by various approaches/models. The *ab initio* approaches are represented by the first four entries from the left: coupled-clusters singles and doubles (CCSD), coupled-clusters singles, doubles, and first-order triples (CCSDT-1), the IM-GCM (IMSRG+GCM), and perturbation theory within the shell model (RSM). VSIMSRG is a valence-space version of the IMSRG that is also an ab initio approach. The rest are the predictions of phenomenological models: the quasiparticle random-phase approximation (QRPA), energy-density functional theory (EDF), the shell model in a pf valence space (SM (pf)), the shell model in the same space with perturbative corrections to the decay operator (SM (MBPT)), and the shell model in the larger $sdpf$ model space (SM (sdpf)).

available) are in the second column of Fig. 6. The gray band lies between the numbers produced by considering excitations of the spherical nucleus ^{48}Ca and those produced by considering excitations of the deformed nucleus ^{48}Ti, the daughter in the decay. Benchmarks against the NCSM in light nuclei (Sec. (D)) showed that the exact result was always between these two kinds of predictions, though usually closer to the smaller one. Thus, the matrix element is consistent with that from the IM-GCM but may ultimately be a little smaller. We can expect the contact term to increase the coupled-clusters matrix element, as it did the IM-GCM matrix element.

The coupled clusters approach can produce a complete set of states in the intermediate nucleus ^{48}Ca, and so has the advantage of being able to calculate the matrix elements for $2\nu\beta\beta$ decay as well as for $0\nu\beta\beta$ decay. Our paper nicely reproduced the measured $2\nu\beta\beta$ decay rate when the energy denominator, on which the rate depends, contained the measured Q value.

One goal we did not achieve was the assignment of systematic error bars. Though both the IM-GCM and coupled clusters papers provide error bars, those mostly reflect simple uncertainties in the effects of model-space extrapolation, oscillator-parameter choice, χEFT fitting prescription, etc. The most important unfinished task is a convincing assessment of systematic uncertainty associated with each many-body method.

^{76}**Ge:** The IM-GCM can be applied to heavier nuclei as well, and we are now (post-DBD) computing the matrix element for the decay of ^{76}Ge, currently used in the LEGEND experiment [54]. That nucleus is computationally difficult, however, because its ground state is triaxially deformed. Projection of mean-field states onto those with well-defined angular momentum is thus much more time consuming, and jobs that carry out the projection in what we hope is a sufficiently large model space are still running. We do have preliminary results in a smaller space, however; they appear in Ref. [55].

The UT group does not yet have a triaxial-basis coupled clusters code and so a calculation would have to be based on a less-than-perfect Hartree-Fock starting point. A triaxial code is only a matter of time, however.

The LLNL group, while not trying to obtain a realistic matrix element, did work towards quantifying the uncertainties in ^{76}Ge matrix elements coming from the truncation of the chiral expansion of the nuclear interaction and currents. To do so, they developed a computationally simple surrogate model consisting of four-nucleon droplets that mimic the valence nucleons in nuclear ground states They used the surrogate to sampled a joint distribution of chiral interactions and operators that was informed by nucleon-nucleon scattering data and the expectations of χEFT. The result is that the chiral truncation errors should lead to uncertainties of only about 30% in *ab initio* matrix elements.

^{130}Te, ^{136}Xe, ^{150}Nd, Etc.: Most of these nuclei are not as complicated as ^{76}Ge, but they are larger and so will require a similar level of computation time (and perhaps more memory). An additional issue arises in such heavy isotopes, however: χEFT interactions are mostly untested there. A reliable $\beta\beta$ calculation in these nuclei must therefore accompany others that reproduce more familiar observables.

(G) Related Work in Nuclei Used in Experiment

The CMU group carried out shell model calculations with phenomenological interactions and operators, and also worked to to develop shell model-like techniques that use *ab initio* effective interactions and operators. One development was an isospin-breaking formalism for use with *ab initio* Hamiltonians. Another was work on the GCM [46], mentioned in the benchmarking section, that was crucial for the development of the IM-GCM discussed just above. The group's work on heavy-particle exchange in $0\nu\beta\beta$ matrix elements, described briefly in the Sec. (B), also isolated theories in which short- and long-range contributions do not interfere with one another [10].

The CMU group examined some more novel issues as well. For the future, when experiments are more sensitive, they analyzed the two-electron opening-angle dependence associated with long and short-range exchange [9]. They also looked at the possibility of electron-cloud-induced oscillations of the virtual neutrino exchanged in $0\nu\beta\beta$ decay [56]. The effects are negligible, but could be more important when (hypothetical) particles called Majorons are emitted during the decay.

The SDSU group, besides working to improve the GCM [47], also developed the shell-model code BIGSTICK so that it can compute $\beta\beta$ matrix elements in large model spaces. Finally, the UNC group and collaborators showed that the addition of isoscalar $l = 1$ bosons to $l = 0$ and 2 bosons improved the fidelity of the interacting boson model to its shell-model underpinnings and would likely improve the accuracy of its predictions

[57, 58].

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