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Towards precise and accurate calculations of neutrinoless double-beta decay

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Abstract

We present the results of a National Science Foundation Project Scoping Workshop, the purpose of which was to assess the current status of calculations for the nuclear matrix elements governing neutrinoless double-beta decay and determine if more work on them is required. After reviewing important recent progress in the application of effective field theory, lattice quantum chromodynamics, and *ab initio* nuclear-structure theory to double-beta decay, we discuss the state of the art in nuclear-physics uncertainty quantification and then construct a roadmap for work in all these areas to fully complement the increasingly sensitive experiments in operation and under development. The roadmap includes specific projects in theoretical and computational physics as well as the use of Bayesian methods to quantify both intra- and inter-model uncertainties. The goal of this ambitious program is a set of accurate and precise matrix elements, in all nuclei of interest to experimentalists, delivered together with carefully assessed uncertainties. Such calculations will allow crisp conclusions from the observation or non-observation of neutrinoless double-beta decay, no matter what new physics is at play.

Keywords: neutrinoless double-beta decay, effective field theory, lattice quantum chromodynamics, *ab initio* nuclear-structure theory, Bayesian uncertainty quantification, Bayesian model mixing

(Some figures may appear in colour only in the online journal)

1. Introduction

In recent years the search for new fundamental physics, for the forces and particles that underlie the Standard Model, for the explanation of the excess of matter over antimatter and

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similar mysteries, and for the sources of symmetries and their violation, has moved increasingly to low-energy experiments. Among the most visible and promising are those that seek to observe neutrinoless double-beta ($0\nu\beta\beta$) decay, a process in which two neutrons inside an atomic nucleus turn into protons, emitting two electrons and no neutrinos. An observation of this process would show that lepton-number is not conserved and that the neutrino mass has a Majorana component, implying that the mass eigenstates are self-conjugate [1]. Observation of $0\nu\beta\beta$ decay would thus provide crucial information about neutrino mass generation [2–4], and suggest that the matter-antimatter asymmetry in the Universe originated in leptogenesis [5]. The major implications of an observation made the construction of a ton-scale $0\nu\beta\beta$-decay experiment the top priority for new projects in the 2015 Nuclear Science Advisory Committee Long Range Plan [6], which set the decadal priorities for nuclear physics in the United States. The anticipated investment is in the range of US$250–400 million.

Smaller experiments already put stringent limits on the decay rate [7–18], e.g. $T^{0\nu}_{1/2} > 2.3 \times 10^{26}$ year for the decay of ^{136} Xe [19]. The next very few years will see stricter limits from experiments that are currently operating or under construction, such as LEGEND-200, CUORE, KamLAND-Zen 800, and SNO+. On a slightly longer time scale, ton-scale experiments [19–24] based on ^{76}Ge, ^{100}Mo, ^{136}Xe, and perhaps other isotopes will come online. The goal of these large experiments is the ability to detect any decay caused by the exchange of light Majorana neutrinos if the neutrino mass hierarchy is inverted (i.e. if the neutrino with the largest electron-flavor component is the heaviest), as well as increased sensitivity to decay caused primarily by the exchange of other still-hypothetical particles.

In order to extract the effective light-neutrino Majorana mass $m_{\beta\beta} \equiv |\sum_i U_{ei}^2 m_i|$ (with m_i the mass of the neutrino mass eigenstate i and U_{ei} the elements of the Pontecorvo–Maki–Nakagawa–Sato matrix) from any of these impressive experiments, one needs nuclear matrix elements (denoted by $M_{0\nu}$) of the decay operators. The degree to which ton-scale experiments will be sensitive to decay caused by the exchange of inverted-hierarchy light neutrinos depends on these nuclear matrix elements, as does the extent to which experiments in more than one isotope will prove useful. The nuclear matrix elements suffer at present from sizable uncertainties [25]. *Their accurate computation, with a quantified uncertainty, is therefore an important task.*

The need for precise nuclear matrix elements is in fact more general than the notion that the exchange of light Majorana neutrinos causes $0\nu\beta\beta$ decay. That idea is based on the assumption that lepton-number violation originates at very high energies and manifests itself in the decay through the 'high-scale seesaw,' which leaves Majorana neutrino masses as its only remnant at low energies. If that is indeed the case, $0\nu\beta\beta$ decay and neutrino-oscillation experiments will together tell us most of what we can learn. High-scale LNV is only one scenario, however, and even in the restricted class of seesaw models, it applies only if the new particles are very heavy right-handed neutrinos. In many Beyond the-Standard Model (BSM) scenarios, other lower-scale sources of LNV can also induce $0\nu\beta\beta$ decay. In left-right symmetric models, for example, heavy neutrinos and charged scalars with TeV-scale masses can be exchanged. In other scenarios there may be light right-handed (sterile) neutrinos with masses much lower than the electroweak scale. The large number of ways in which the lepton-number could be violated (see, e.g. [26] for a review) means that ton-scale searches for $0\nu\beta\beta$ decay have a significant discovery potential beyond the inverted-hierarchy high-scale seesaw. Each kind of LNV leads to its own set of transition operators, the nuclear matrix elements of which must be calculated. If the calculations are sufficiently accurate, we can assess the sensitivity of the generation of experiments now coming online to various kinds of LNV. We can also provide a subsequent generation of experiments with information on how best to narrow the range of possibilities for LNV and neutrino mass generation through

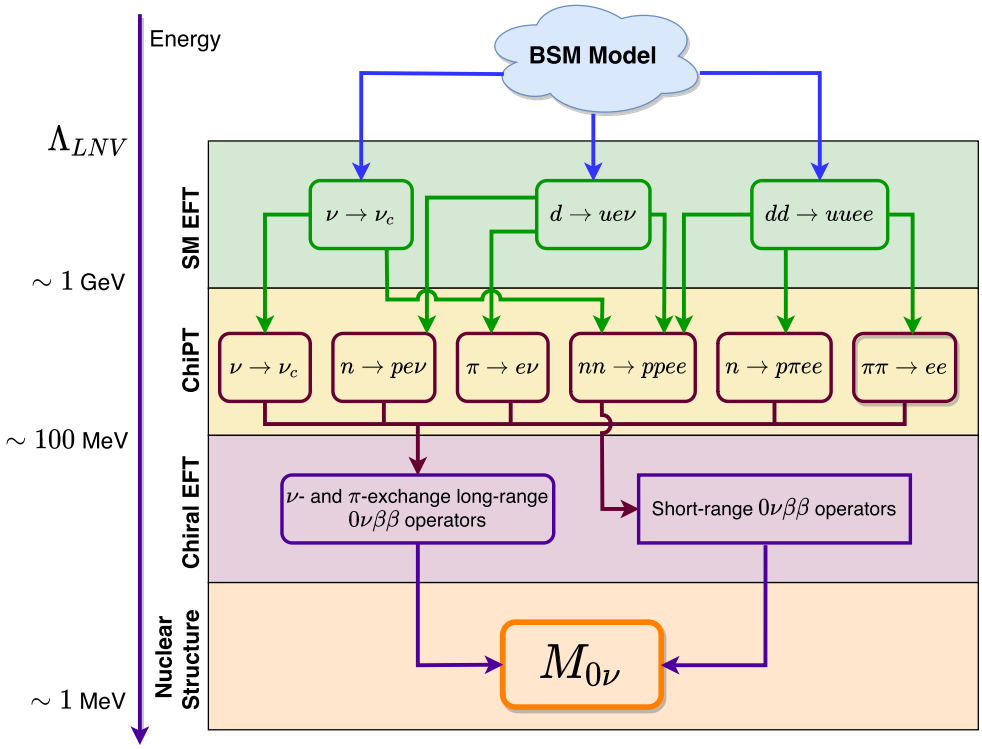

Figure 1. A 'tower of theories' leading to the computation of the nuclear matrix elements $M_{0\nu}$ that control the rate of $0\nu\beta\beta$ decay. At the highest level, above the cutoff Λ_{LNV} for all effective theories, is the ultimate BSM LNV. It manifests itself at the quark and gluon level through Standard-Model EFT, at the nucleon and pion level through chiral perturbation theory (ChiPT), at the nucleon-only level (i.e. with pions no longer part of the Hilbert space, but instead accounted for in multi-nucleon operators) through chiral-EFT, and at the nuclear level through the techniques of nuclear-structure theory. Figure adapted from [27].

measurements of single-electron spectra, electron angular distributions, and the isotopic dependence of the decay rate.

The ability to compute all the relevant nuclear matrix elements requires work at widely separated energy scales, from the high energies at which LNV originates all the way down to nuclear energies, and the ability to bridge the scales. Effective Field Theory (EFT) provides the bridge by expanding observables and Lagrangians in the ratios of the important energy scales. In reality the calculation is done via a series of EFTs—a connected set of bridges rather than a single one; see figure 1 for an illustration. The Standard Model EFT (SM EFT) allows us to encode the effects of different LNV mechanisms in operators involving neutrinos, electrons, and d and u quarks, thereby taking us from the TeV scale to the scale of quark confinement at around 1 GeV. Converting these operators into hadronic operators that are organized through chiral perturbation theory requires non-perturbative input from lattice QCD (LQCD). Chiral perturbation theory operators are then used to derive operators in a nucleons-only Hilbert space; following that step, the operators can be used in many-body calculations of nuclei. Taken together the bridges deliver, for each LNV source, a separate and specific set of chiral-EFT $nn \to pp$ transition operators that can then be used in nuclear

many-body calculations. The combination of SM EFT, LQCD, chiral-EFT, and *ab initio* (first-principles) nuclear many-body methods, each of which has the ability to control uncertainty, therefore provides a path—the only path, in fact—toward the reliable estimation of uncertainties in $M_{0\nu}$.

Chiral-EFT is key to the progress made to this point, and to future efforts to quantify uncertainties. Chiral-EFT [28–31] is the extension of chiral perturbation theory to the few-nucleon problem. Just like chiral perturbation theory, chiral-EFT is organized as an expansion in powers of p/Λ or m_π/Λ, where p is a typical nucleon momentum, m_π is the pion mass and Λ is the theory's 'breakdown scale' of about 500 MeV. But chiral-EFT is not a perturbative theory, because it has to account for nuclear binding. Although discussions of exactly how to do that continue (see, e.g. [32]) chiral-EFT has the virtue of delivering consistent nuclear forces and $0\nu\beta\beta$ operators up to a given order in the chiral-EFT expansion. Even better, these operators include the consequences of QCD's chiral symmetry, e.g. connections between pionic operators and the axial current that governs beta decay. Perhaps most significantly for the purposes of this document, chiral-EFT permits estimation of the uncertainty associated with the model of the nuclear force and the interactions that govern $0\nu\beta\beta$ decay. A kth order chiral-EFT calculation should have a fractional error of $O(\{p, m_\pi\}^{k+1}/\Lambda^{k+1})$. It follows that different implementations of chiral-EFT—different orders of the calculation, different regulator choices—should give answers that are consistent with one another once this error estimate is taken into account. Bayesian techniques have recently been employed to quantify this error [33], and show that—if the chiral-EFT calculation is implemented carefully—the error estimate provides a good account of the predictive accuracy of chiral-EFT in light nuclei [34, 35]. Chiral-EFT forces and operators, therefore, provide the starting point for *ab initio* calculations that use the nuclear many-body methods described below.

The nuclear-theory community has made significant progress, at all the levels in this tower of EFTs, toward more accurate calculations of $M_{0\nu}$. But the progress has in part served to confirm that there are $O(1)$ uncertainties in $M_{0\nu}$. These uncertainties (unless reduced) will prevent us from learning about the sources of LNV, even if several experiments detect the process.

There is therefore still much to do. In particular:

- The $0\nu\beta\beta$ transition operators used in nuclear-structure physics are now written in terms of 'low-energy constants' (LECs) that multiply terms in the chiral-EFT Lagrangian that is used at the hadronic scale. In chiral-EFT, the LECs multiplying the terms at the lowest orders are thus the most important. Previously unrecognized LECs associated with zero-range $nn \to pp$ transition operators appear even at leading order in the $0\nu\beta\beta$ piece of the chiral Lagrangian, for both light Majorana neutrino exchange [36] and TeV scale LNV [27]. We must improve our knowledge of these LECs, both by relating $0\nu\beta\beta$ decay to other $\Delta I = 2$ processes and by direct calculation within LQCD.
- To use the results of EFT and LQCD in the computation of nuclear matrix elements—that is, to use the chiral-EFT Hamiltonians and transition operators that these methods supply in many-body calculations—we need to improve *ab initio* methods. The improvement will involve an increase in accuracy, the use of a wide range of chiral-EFT Hamiltonians (to allow uncertainty quantification), and a careful analysis of the way such methods employ the EFT operators. The first two of these will require, in addition to analytic work, more efficient use of our best supercomputing resources. Existing codes and their extensions will need to be reworked to leverage accelerators such as GPUs. Benchmarking with methods that are known to give very accurate results (so-called

'quasi-exact' methods that have thus far been restricted by complexity to light nuclei) is also important.
- At both the hadronic and nuclear scales, we need a consistent and unified quantification of uncertainties. We must be able to both propagate parameter uncertainties to observables and to account for and disentangle deficiencies in our calculations. The innovative use of Bayesian methods will be essential.

In short, the framework developed in the last few years to combine LQCD, EFT, and *ab initio* nuclear structure is not yet efficient enough to allow a genuine assessment of uncertainty. To be of real use in the search for new physics, all three ingredients must be improved in the coming decade and made more computationally efficient; their uncertainty also needs to be reliably addressed. But these kinds of intelligent improvements will not, on their own, be enough: increased access to computing resources and dedicated exascale allocations will also be important.

Some of these issues have been discussed recently. A Snowmass white paper [37] provides a particle-physics perspective, and [38] reviews both the nuclear and particle theory of $0\nu\beta\beta$ decay alongside the experimental situation. This paper differs from those in focusing tightly on modern methods of nuclear theory and on uncertainty quantification, and in particular on the improvements that will allow accurate values for $M_{0\nu}$with meaningful error bars, for any particular BSM mechanism.

In the next section, we provide a summary of the current state of-the-art in both the nuclear-physics aspects of $M_{0\nu}$ (section 2.1) and uncertainty quantifcation (UQ) in nuclear theory (section 2.2). Section 3 then discusses the innovations and calculations that are needed to advance the nuclear theory of $M_{0\nu}$, while section 4 describes a plan to quantify uncertainty in those calculations. Because of the significant emphasis on UQ for $0\nu\beta\beta$ matrix elements in this paper, sections 4 and 2.2 are quite detailed and explicit about how we think that UQ can be carried out. We close in section 5 with a summary of the theoretical advances and collaborative structures that are needed in order to establish precise and accurate calculations of neutrinoless double-beta decay.

2. Summary of the current state of the art

2.1. Physics

Much of the current state of the art in the computation of $M_{0\nu}$ arose from work in the recent DOE-funded DBD topical theory collaboration on nuclear theory for double-beta decay and fundamental symmetries [39]. LQCD, EFT, and nuclear many-body methods all played a role in this effort to solve the multi-scale problem of nuclear $0\nu\beta\beta$ decay. We discuss recent developments in each of these areas.

EFT. Until recently, the connection of nucleon operators with fundamental sources of lepton-number violation tended to be ad hoc, with BSM models analyzed individually and unsystematically. The first application of the framework of chiral-EFT to the problem, for $0\nu\beta\beta$ decay induced by heavy-particle exchange, appeared in [40]. In the last few years, work of this kind has grown much more systematic. References [27, 41, 42] systematized the work of [40], showing how the parameters that determine the rates of a very heavy-particle lepton-number-violating physics work their way down into nucleon-level $\beta\beta$ operators. At around the same time, [43] treated light-neutrino exchange, showing that working to N^2LO requires 'non-factorizable' diagrams (those that cannot be broken in two by cutting the line representing the exchanged neutrino) that had never been considered before. Shortly after that,

researchers made the surprising discovery [36] that a contact interaction, representing the effects of high virtual-neutrino momenta that are integrated out of the chiral-EFT, occurs at the leading order. Though the coefficient of the contact operator was initially unknown, it was later determined approximately through a resonance-model-based interpolation between perturbative QCD and low-energy pion and nucleon dynamics. [44, 45]. For the first time, nuclear many-body computations of $M_{0\nu}$ in the nuclei used in experiments are taking the contact term into account. So far it has caused all *ab initio* matrix elements to increase.

LQCD. The hope is that LQCD will soon be able to directly supply the coefficient of the aforementioned contact term, as well all other relevant LECs. In the last few years, the field has made significant progress toward that goal. A contribution to $0\nu\beta\beta$ decay with TeV-scale LNV is produced by the exchange of BSM heavy particles between two pions, each of which are then absorbed by protons as they turn into neutrons. The exchange between these virtual pions is easier to compute with LQCD than the direct exchange between nucleons, and in recent work the dependence of the resulting $0\nu\beta\beta$ nucleon-level matrix elements on parameters that specify BSM models has been calculated [46, 47]. Pionic matrix elements in the light-neutrino exchange scenario have also been computed in LQCD, and the corresponding LECs in chiral perturbation theory have been constrained [48, 49]. Progress toward direct calculations of $nn \to pp$ matrix elements will come soon, and the formalism for constraining contact LECs from future LQCD calculations is being developed [50, 51].

Nuclear Structure. At the nuclear-structure scale, recent progress has been mostly in applying newly developed non-perturbative *ab initio* many-body methods to $\beta\beta$ decay. Such 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 produce (approximate) solutions to the Schrödinger equation in heavier nuclei. Three distinct *ab initio* methods have been applied together with chiral-EFT interactions to the heavy open-shell nuclei of interest for $0\nu\beta\beta$ experiments. The first two, the in-medium generator coordinate method (IM-GCM) and the valence space IMSRG (VS-IMSRG) are variants of the In-Medium Similarity Renormalization Group (IMSRG), an approach in which one uses renormalization-group flow equations to decouple a predefined 'reference' state, ensemble, or subspace from the bulk of the many-body Hilbert space. The third method is Coupled Cluster (CC) Theory; it uses an ansatz for the ground state in which particle-hole excitation operators are exponentiated before being applied to a Slater determinant. It also decouples a reference state, albeit via a similarity transformation that results in a non-Hermitian Hamiltonian.

All three of these methods, along with many more phenomenological schemes, have been applied to the computation of $M_{0\nu}$ for light-neutrino exchange in ^{48}Ca, the lightest isotope that can be used in an experiment, and the Valence Space IMSRG has been applied to heavier isotopes. Figure 2 displays the compiled results for ^{48}Ca. Those produced by the methods just described—the 'most *ab initio*'—are shown in green on the right of the figure. The uncertainty range is more significant for these than for other methods, but still omits most systematic error.

The next section reviews the state of the art in uncertainty quantification. The rest of this document then discusses both the ways in which physics methods can be improved in accuracy and the ways in which remaining uncertainty in their predictions for $M_{0\nu}$ can be reliably estimated.

2.2. Uncertainty quantification

In 2011 *Physical Review A* published an Editorial that stated '…there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting

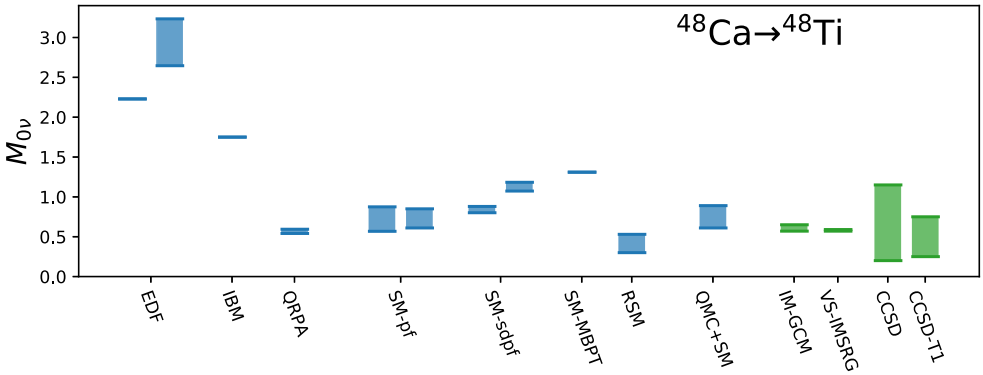

Figure 2. The light-neutrino exchange $M_{0\nu}$ for the transition ^{48}Ca→^{48}Ti, is computed in various approaches. The four right-most values, in green, all result from the same chiral-EFT interaction. References: EDF [52, 53], IBM [54], QRPA [55], SM-pf [56, 57], SM-sdpf [58], SM-MBPT [59], RSM [60], QMC+SM [61], IM-GCM [62], VS-IMSRG [63], CCSD, CCSD-T1 [64].

the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable.' [65]. Uncertainty quantification is crucial for calculations of $0\nu\beta\beta$-decay in nuclei. The planning and—eventually, we hope—the interpretation of $0\nu\beta\beta$-decay measurements requires that theorists deliver not just an expectation value for $M_{0\nu}$, but also an uncertainty that represents the range of probable values that matrix element can take and does so in a statistically meaningful way. The goal of the uncertainty quantification (UQ) is not a precise evaluation of whatever is missing from the calculation. Quoting again from [65]: "The aim is to estimate the uncertainty, not to state the exact amount of the error or provide a rigorous bound."

UQ in nuclear-physics calculations pre-dated that Editorial but standard regression analysis was prevalent for many years [66]. Since then, nuclear-theory UQ has become much more sophisticated. This progress has taken place on several fronts.

The first, and most straightforward kind of UQ, is the estimation of error bars on the parameters $\boldsymbol{\theta}$ in the nuclear-physics model being employed, then the propagation of those uncertainties—including their correlations—to model predictions. An early example of such an effort is the estimation of the parameters in a sophisticated nuclear energy-density-functional [67]. There are many recent examples of nuclear-structure calculations that do this, but a particularly striking one from the *ab initio* world constrained the parameters of nuclear forces using data from light nuclei and propagated the resulting uncertainties to predictions for properties of ^{208}Pb [68].

Three pieces of theory technology are commonly employed in such studies:

- Bayes' theorem, which relates the multi-dimensional posterior probability density p of the model parameters θ to the data, y, used to constrain those parameters, according to:

$$p(\theta|y) \propto p(y|\theta)p(\theta), \tag{1}$$

  where $p(\theta)$ is the *a priori* distribution of the parameters θ.
- A method by which a representative set of samples of the posterior probability distribution $p(\theta|y)$ can be obtained. Markov Chain Monte Carlo (MCMC) sampling is commonly employed, and was combined with a technique called 'history matching' in [68]. We note that with such a set of samples in hand, it is conceptually straightforward to

obtain a predictive probability distribution for, say, $M_{0\nu}$. That distribution is found by repeated forward evaluation of the model for $M_{0\nu}$ at the different parameter values θ in the set of samples.

- Emulators that allow rapid evaluation of the (approximate) model at different values of the parameters θ. This makes practical the computation of the likelihood $p(y|\theta)$ within whatever sampling framework is chosen.

Nuclear theorists have also become more attuned to the imperfections in their models. The inclusion of a 'model discrepancy' term in the analysis of data is known to be crucial for accurate parameter estimation [69, 70]. This means that one must admit that not just data, but also calculations, have imperfections that may cause a mismatch between theory and experiment. This idea can be formalized as

$$y_{\rm exp}(x) = y_{\rm th}(x;\,\theta) + \delta y_{\rm exp}(x) + \delta y_{\rm th}(x), \tag{2}$$

where the last two terms encode, respectively, the experimental error (often taken to be independent at the x's corresponding to different data y) and the theory uncertainty (which is almost certainly *not* independent, i.e. we expect to be correlated across different x's). Significant effort has gone into building models of $\delta y_{\rm th}$ for EFT calculations [33, 71]; since EFT methods are characterized by a systematic expansion in a small parameter, one can predict how they will fail and so write down candidate functional forms for $\delta y_{\rm th}$. But, even when such control is not available, model defects can still be productively introduced, e.g. Gaussian processes can be used to model the discrepancy between density-functional-theory calculations of masses and experimental data thereon [72].

Ultimately, though, the complex dynamics of nuclei means that different theoretical models will be employed to describe them. This diversity of models is advantageous because the methods have complementary strengths but also different systematic model discrepancies. This becomes a virtue by exploiting the third area of progress, which has been in the use of forms of Bayesian model averaging (BMA) or Bayesian model mixing (BMM) to incorporate insights from different models into a unified prediction in a statistically rigorous way. BMM can only be done reliably if individual models $\mathcal{M}_k$ have had their uncertainties quantified in the ways described in the previous two paragraphs. Once that has taken place, the predictions of those models for the observable of interest y^* can be weighted according to 'scoring criteria':

$$p(y^*|y,\,y_{ev}) = \sum_k w_k(y_{ev}) p(y^*|y,\,\mathcal{M}_k). \tag{3}$$

Here, $p(y^*|y,\,\mathcal{M}_k)$ is the posterior for the observable y^*, given the data y, in a particular model $\mathcal{M}_k$, and $w_k(y_{ev})$ is a weight that is determined by the model's performance on a target (or evidence) dataset, y_{ev}. While in the BMA expression (3) the weights are constant across the domain, in the more advanced BMM they can also depend on x. We pause here to make two crucial points:

- The data, y_{ev} that are used to assess the aspects of model performance that are pertinent for predicting y^* need not be the same as the dataset(s) used to calibrate the models. Ideally, the data y_{ev} will be chosen because they are understood to be, or analyzed to be, a good proxy for the quantity of interest, y^*, i.e. models' ability to predict y^* is highly correlated with their ability to predict whatever observables are selected to be part of y_{ev}.
- We note that that performance will almost certainly be addressed within the context of the model discrepancy $\delta y_{\rm th}$ of each model, and hence an understanding of those model discrepancies plays a critical role in between-model UQ.

Early nuclear-physics applications of model averaging can be found in [73, 74].

In 2020, the Bayesian analysis of nuclear dynamics (BAND) collaboration [75] began its effort to lower the barrier for nuclear theorists to perform all three of these types of uncertainty quantification. A particular interest within BAND is methodological work on BMM. The main product the collaboration seeks to deliver is software packages and use cases that facilitate emulation, model calibration, and model mixing. The goals of BAND are described in [76].

Within the DBD Topical Collaboration, some ideas were proposed to quantify the uncertainties in calculations of *ab initio* $M_{0\nu}$. However, the implementation of these ideas was limited by the inability to rapidly evaluate these matrix elements for the nuclei of interest in $0\nu\beta\beta$ experiments. This made it difficult to even accomplish the first, parametric, kind of UQ. The determination of model discrepancy for the different many-body methods employed in $0\nu\beta\beta$ studies remains a topic of forefront research, see section 4.

3. Physics progress required

Future work in the community to deliver reliable $0\nu\beta\beta$ nuclear matrix elements will probably focus on advancing LQCD and EFT calculations of the underlying matrix elements in the few-nucleon sector, and *ab initio* nuclear many-body calculations that use the LQCD and EFT input in experimentally relevant isotopes. We discuss these subjects in this section and lay out a path for rigorous UQ in the next section.

3.1. Lattice QCD and EFT

The goal of a combined EFT and LQCD effort in the $0\nu\beta\beta$ program will be the identification and computation of the LECs multiplying $nn \to pp$ transition operators in chiral-EFT. Because LNV originally involves leptons and quarks, one has to evaluate matrix elements of quark operators in hadronic states in order to link LNV parameters such as $m_{\beta\beta}$ to the LECs. The program of constructing consistent and predictive nuclear EFTs has a long history and a recent review summarizing its status and prospects can be found in [31].

As mentioned in section 2.1, analyses of the $0\nu\beta\beta$ amplitude revealed that a new $nn \to pp$ contact interaction is needed at leading order in chiral-EFT, even for light Majorana neutrino exchange [36, 43]. The associated LEC, called g_ν^{NN}, is not determined by symmetry considerations or experiment (at least not in a straightforward way) and so must be obtained theoretically. The LEC g_ν^{NN} has been studied so far by applying both large-N_c and dispersive methods, while LQCD studies require methods that are still under development. Large-N_c QCD [77] relates g_ν^{NN} to LECs that can be extracted from the charge-independence-breaking combination of nucleon-nucleon scattering lengths in the $^1S_0$ channel. Meanwhile, the dispersion-theory approach, inspired by the Cottingham formula for electromagnetic hadron masses [78, 79], leads to a prediction for the $nn \to pp$ amplitude near threshold, from which g_ν^{NN} can be extracted in any EFT regularization and renormalization scheme, including those used in nuclear many-body theory (see [80] for an early use of this $nn \to pp$ input in *ab initio* nuclear many-body calculations). The main uncertainty in this approach comes from inelastic intermediate states that can appear between the two insertions of the weak current (e.g. $NN\pi$ states). The existing estimates of g_ν^{NN} can be improved by analyzing suitable $\Delta I = 2$ observables, thus anchoring g_ν^{NN} to data. Finally, as discussed below, LQCD can play a major role in a first-principles determination of g_ν^{NN} [51, 81, 82].

The leading order LECs associated with TeV-scale LNV operators are currently completely unknown. Their determination will be possible through the use of dispersion-theory techniques similar to those developed in [78, 79], as well as by a direct calculation in LQCD. In fact, direct LQCD calculations can in principle determine the entire $nn \to pp$ amplitude (see [83, 84] for recent reviews of the role of LQCD in constraining nuclear observables). The interplay between LQCD and EFT is symbiotic. On the one hand, matching EFT and LQCD will enable an assessment of the theoretical foundation of nuclear EFT and a calibration of its truncation scheme. On the other hand, EFT descriptions allow better quantification of the systematic uncertainties in LQCD calculations, providing reasonable extrapolation forms for taking continuum and infinite-volume limits. Furthermore, in order to play a role in the $0\nu\beta\beta$ program, LQCD calculations need to be performed at quark masses that are sufficiently close to the physical values to allow reliable extrapolations to the physical point. Such extrapolations rely on EFTs, which in turn rely upon LQCD input to determine the relevant LECs. Thus, an interplay between LQCD calculations of two-nucleon (NN) observables and EFT will be necessary to determine at which quark masses one may trust results for $0\nu\beta\beta$-decay observables.

Before calculating the $nn \to pp$ amplitudes with LQCD, however, the low-energy spectra and scattering amplitudes in the NN system need to be calculated with precision. Doing so allows one to determine which operators couple sufficiently well to the ground states of interest, to understand the systematic uncertainties inherent to NN systems, and to match finite-volume Euclidean matrix elements to infinite-volume transition amplitudes. The NN studies to date have been largely carried out at very large quark masses, where extrapolation to the physical point cannot be controlled. Fully understanding the systematic uncertainties will become even more crucial as the quark masses are lowered toward their physical values because of a signal-to-noise problem for nucleons, in which statistical noise grows exponentially with the pion mass, atomic number, and Euclidean time [85–87]. Furthermore, in calculations at lighter quark masses (which require larger lattice volumes), the energy gaps that dictate the exponential decay of excited states with Euclidean time become very small, causing a slow approach to the ground state that may be obscured by the growth in noise. Thus, improved operators, analysis, and understanding of excited-state contamination are of critical importance.

These complications mean that LQCD still cannot demonstrate that two nucleons form bound states, even at large quark masses that make precise calculations easier. Recent work within the LQCD community has highlighted the importance of fully-controlled calculations in the NN sector. First, the use of improved interpolating-operator sets and analysis techniques based on the variational principle of quantum mechanics has led to results [88–90] that cast doubt on earlier spectroscopy calculations at similar quark masses. Second, a preliminary study of the discretization effects of two-baryon calculations has shown large shifts in the binding energies away from the continuum limit [91]. The latter finding, in particular, needs to be verified by different groups with different lattice actions, and may indicate that NN calculations must be performed at multiple fine lattice spacings. This would significantly increase the cost of calculations.

To use LQCD to access the $0\nu\beta\beta$ amplitude, one needs to develop indirect mapping relations. This is because the notion of asymptotic states is absent in the finite Euclidean spacetime that is used in the LQCD setting. A general mapping exists to obtain matrix elements of local (short-range) operators such as those appearing in the high-scale models of $0\nu\beta\beta$ decay within two-nucleon states [50]. As an input, this mapping requires two-nucleon spectra and the energy dependence of elastic scattering amplitudes. The existing mapping for the matrix element associated with light-neutrino exchange involves a matching to the leading

order nucleonic EFT [51] and requires as input the two-nucleon spectra and scattering amplitudes. The mappings for such long-range matrix elements are in general more complex than those for local matrix elements because a straightforward analytic continuation in the presence of on-shell intermediate states is not possible [92–95]. With properly infrared-regulated neutrino propagators, however, analytic continuation will be straightforward in future calculations of the $0\nu\beta\beta$ amplitude [48, 49]. Techniques for computing both the short- and long-distance contributions to $0\nu\beta\beta$ processes have already been developed and applied in studies of the $\pi^- \to \pi^+ e^- e^-$ and $\pi^- \pi^- \to e^- e^-$ processes [46, 48, 49], which also constrain pionic contributions within nuclear $0\nu\beta\beta$ decays. Calculations of the $nn \to ppe^- e^-$ process will be significantly more involved for the reasons discussed above, but will be a crucial next step.

With the broad goal of achieving a systematic quantification of nuclear uncertainties, we must face the challenges of extending the analysis of the $0\nu\beta\beta$ transition operator beyond leading order in chiral-EFT, especially in the case of light-neutrino exchange. We must also go beyond two-nucleon observables to reliably determine the role of multi-nucleon effects in double-beta decay. Regarding the $nn \to pp$ amplitude, both in Weinberg's power-counting (WPC) and in renormalized chiral-EFT, the first corrections arise at next-to-next-to-leading order ($\mathrm{N^2LO}$) [96]. In the two-body sector, the transition operator includes contributions from the nucleon vector, axial, and induced pseudoscalar form factors (which are customarily included in nuclear calculations), from pion-neutrino loops [43], and from new contact interactions required to absorb the divergences in these loops. These include the couplings of two electrons to two pions ($g_\nu^{\pi\pi}$), to two nucleons and one pion ($g_\nu^{\pi N}$), and to four nucleons (a correction to g_ν^{NN}). $g_\nu^{\pi\pi}$ is well determined by LQCD [48, 49], while extracting the correction to g_ν^{NN} will require the matching of LQCD and chiral-EFT amplitudes at higher orders. The short-range structure of the two-body $0\nu\beta\beta$ operator at $\mathrm{N^2LO}$ is at the moment unknown beyond WPC. Reference [96] pointed out that the promotion of g_ν^{NN} to LO implies that certain derivative operators in the spin-singlet channel are also more important than in WPC, but a full analysis of the LNV scattering amplitudes to $\mathrm{N^2LO}$ does not yet exist, and needs to be developed to interpret anticipated LQCD results. A deeper question is whether the chiral and momentum expansions of chiral-EFT converge (and converge to what is observed in Nature). This question is open even for single baryons [84, 97] and relatively light systems [98–100], and needs to be answered as the community moves beyond purely phenomenological approaches. LQCD input for the unknown LECs at successively higher orders can help resolve power-counting questions for LNV processes.

Moving to the question of multi-nucleon corrections, we note that two-body currents, which are important in the g_A-quenching problem in β decays [101, 102], first contribute to $0\nu\beta\beta$ decay at $\mathrm{N^2LO}$, by generating three-body corrections to the operator. These corrections were considered in [103, 104] and found to be compatible with power-counting estimates. Furthermore, in the three-body sector, a goal for the chiral-EFT community is to validate or falsify WPC's expectations, by studying suitable few-body amplitudes. Once calculations of two-body transitions have been achieved with systematic control, LQCD studies of $0\nu\beta\beta$ decay of systems with $A = 4$ and $A = 6$, if they can be carried out, will provide valuable additional information. Such calculations can reduce systematic uncertainties in the process of matching $0\nu\beta\beta$ amplitudes to the chiral-EFT used in nuclear many-body calculations. In particular, constraining the same LECs from LQCD calculations of different processes will not only reduce statistical uncertainty, but will also reduce the uncertainties in nuclear EFTs that arise from choices of scheme or regulator. Useful transitions will probably include the $A = 4$ processes ${}^4\mathrm{H} \to {}^4\mathrm{Li}\, e^- e^-$ and ${}^4\mathrm{n} \to {}^4\mathrm{He}\, e^- e^-$, and the $A = 6$ transitions ${}^6\mathrm{He} \to {}^6\mathrm{Be}\, e^- e^-$

(for which nuclear-structure calculations have been performed [105]), and $^{6}\mathrm{H}\to{}^{6}\mathrm{Li}\,e^{-}e^{-}$ (which introduces additional challenges for many-body approaches because ^{6}H is unstable). To reduce the cost of extrapolating such LQCD calculations to infinite-volume, directly matching matrix elements to finite-volume EFT calculations [106–109] may be a valuable approach to precisely determining the LECs.

In summary, while significant outstanding challenges must be overcome to reliably determine the $nn\to pp$ amplitude, for both the light-neutrino exchange and the short-distance $\Delta I=2$ 4-quark operators, there exists a clear roadmap for addressing them. Following it will require a concerted effort in LQCD, EFT, and the coupling of these theories, as well as computing resources at the exascale and beyond, both to quantify the uncertainties in the relevant two-body process and to build an understanding of multi-nucleon corrections.

3.2. Many-body methods

All experimentally relevant $0\nu\beta\beta$ candidate nuclei, with the exception of ^{48}Ca, are open-shell and at least of medium mass. Consequently, only a subset of the currently-available *ab initio* many-body methods can be used to compute the nuclear matrix elements that govern their decay. First computations of the nuclear matrix elements have been performed in coupled cluster theory [64], the IM-GCM [62], and the VS-IMSRG [63]. We describe each of these methods and prospects for improving them next.

3.2.1. Coupled cluster method. In the coupled cluster method [110–112], the exact wave function $|\Psi\rangle$ is parameterized by the exponential ansatz $|\Psi\rangle=\mathrm{e}^{\hat{T}}|\Phi_0\rangle$, where the reference $|\Phi_0\rangle$ is a product state, and the cluster operator $\hat{T}$ generates particle-hole excitations. One expresses $\hat{T}$ in terms of single, double, triple etc particle-hole excitations and (usually) truncates it at the so-called doubles or triples level. This is the main approximation. The calculation of transition matrix elements in coupled cluster theory is complicated by the fact that $\hat{T}$ is purely an excitation operator, i.e. the fact that the similarity transform $\mathrm{e}^{-T}\hat{O}\mathrm{e}^{T}$ of a Hermitian operator $\hat{O}$ is not Hermitian. This implies that the bra version of a state needs to be parameterized through a de-excitation operator rather than an excitation operator. An additional complication for $0\nu\beta\beta$ decay is that the initial and final states are the ground states of different nuclei, with each in principle requiring its own $\hat{T}$ operator and reference state. In practice, one expresses the final state as a generalized excitation of the initial state through the equation-of-motion method as$|\Psi_F\rangle=\mathrm{e}^{\hat{T}}\hat{R}|\Phi_0\rangle$, where $\hat{R}$ is a double-charge-changing excitation operator [64]. Alternatively, one can express the initial state as an excitation of the final state. In the absence of any truncation, these two choices should yield identical results, so the difference between the two is an indication of the truncation error.

Like $\hat{T}$, the excitation operator $\hat{R}$ is expanded in terms of charge-changing few-nucleon 'excitations' and truncated at a doubles or triples level. This approximation may not be accurate when the initial and final nuclei are very different in structure, because, for example, they differ in their intrinsic deformation. Indeed, the spherically-symmetric coupled cluster method works well for computing properties of closed-shell nuclei such as ^{48}Ca. However, the ground state of ^{48}Ti (the final state in the decay of ^{48}Ca) is open-shell and is better treated with an intrinsically deformed (though axially symmetric) reference state, which is computationally more expensive. In benchmarks performed so far [64], it appears that taking $|\Phi_0\rangle$ to be the deformed ^{48}Ti state yields more accurate results, though the reason is not entirely known.

We can expect this approach to be applied to more nuclei and with more accuracy in the next few years. With enough computation time, it can be generalized to allow triaxial

deformation of the reference state (and thus a good calculation, e.g. in ^{76}Ge) and the restoration of rotational symmetry through projection onto states with good total angular momentum [113]. These developments will turn the method into a much more versatile tool for the computation of $0\nu\beta\beta$ nuclear matrix elements.

3.2.2. IM-GCM. The IM-GCM [62, 114] is a combination of the GCM [115] and the MultiReference In-Medium Similarity Renormalization Group (MR-IMSRG) [116, 117] ('Multireference' refers to a generalization of the renormalization-group flow equations to work with a reference state that is more complex than a Slater determinant). The GCM efficiently captures the collective long-range correlations which are important in deformed nuclei, while the MR-IMSRG captures short-range correlations associated with the repulsive core of realistic nuclear interactions.

One can view the IMSRG as a way to generate a unitary transformation U of the Hamiltonian that brings it to a form more amenable to solution. The transformation is parameterized by a flow parameter s, yielding a differential equation for the transformed Hamiltonian $H(s) = U(s)HU^{\dagger}(s)$ and for other consistently-transformed operators $\mathcal{O}(s) = U(s)\mathcal{O}U^{\dagger}(s)$. The unitary transformation, which is conveniently expressed in the Magnus formulation as $U(s) = \mathrm{e}^{\Omega(s)}$ [118], is designed so that with increasing s, a reference state $|\Phi_0\rangle$ increasingly approximates an eigenstate of $H(s)$.

In the IM-GCM, the approach is to take $|\Phi_0\rangle$ to be the ground state of a GCM calculation. The GCM ground state is expressed as a linear combination of configurations $|\Phi(q)\rangle$ labeled by a set of generator coordinates q (e.g. quadrupole deformation), so that $|\Phi_0\rangle = \sum_q f(q)|\Phi(q)\rangle$. The amplitudes $f(q)$ are obtained by minimizing the energy via the Hill–Wheeler–Griffin equation, which amounts to a diagonalization in the space of GCM states $|\Phi(q)\rangle$. As we noted in the context of coupled cluster theory, the initial and final states in any $0\nu\beta\beta$ decay are different, a fact that complicates most computations. The transformations $e^{\Omega_I(s)}$ and $e^{\Omega_F(s)}$ that decouple the initial and final states are different.

In [114], this complication was addressed by combining the IMSRG transformation and GCM calculations for the initial and final states in different ways, again with the understanding that, without approximations, all these combinations should give the same results. In more recent work, a powerful alternative was presented in the form of an ensemble composed of reference states in both the initial and final nuclei that allows one to use a single transformation rather than two separate ones [62].

The main approximation in the MR-IMSRG flow equations is that all operators are truncated at the normal ordered two-body (NO2B) level. In the next few years, with enough computational capacity, we will be able to go beyond this approximation by either exactly or approximately including the effects of three-body operators that are induced by the flow equations. A first step in this direction indicated that the correction due to induced three body operators is sub-leading (on the order of 10% of the NO2B correction) [62, 119]. The result is encouraging, but the corrections are large enough that they should be included.

Another approximation is in the selection of generator coordinates. In principle, one can continue to add more coordinates that are believed to be relevant (for example, proton-neutron pairing gaps) and confirm that the answer does not change, but it is difficult to establish that all important degrees of freedom have been explored. Historically, this has been a significant issue for the GCM calculations based on phenomenological interactions. In the IM-GCM, this issue can be overcome because dependence of the transformation on the flow parameter s offers a powerful diagnostic tool: If sufficient degrees of freedom are included in the MR-IMSRG flow and the GCM basis, the unitarity of the transformation will not be spoiled by truncation errors, and all observables should be independent of s [120, 121].

3.2.3. VS-IMSRG. In the VS-IMSRG [122], as in the IM-GCM, the strategy is to perform a unitary transformation to bring the Hamiltonian into a form more amenable to solution. In this case, the transformation block-diagonalizes the Hamiltonian such that an additional diagonalization in a valence shell-model space yields exact results (assuming no truncations are made in the transformation).

The VS-IMSRG calculations carried out thus far have generally performed the normal ordering with respect to a closed-shell reference state or an uncorrelated 'ensemble' reference that has the correct number of protons and neutrons on average. As with coupled cluster theory, one needs to choose the initial or final state as the reference and, in the absence of truncation, this should not affect the answer. The simpler reference used in the VS-IMSRG (compared to, e.g. the IM-GCM) is somewhat compensated for by the subsequent exact diagonalization in the valence space, resulting in a complementary approximation scheme. Like IM-GCM, the VS-IMSRG as currently practiced truncates operators at the two-body level after normal ordering, and the clear next step is the approximate inclusion of the effects of induced three-body operators. Again, with sufficient computational resources and personpower, this can be done.

3.2.4. Benchmarking with quasi-exact methods. Quasi-exact *ab initio* methods, namely quantum Monte Carlo (QMC) and the no-core–shell model (NCSM), are generally limited to light systems, which are not directly relevant for $0\nu\beta\beta$ experimental searches. They play an important role, however, in benchmarking the methods we have discussed, which can reach the relevant heavier systems. The three methods described above, coupled cluster theory, IM-GCM, and VS-IMSRG, have all been benchmarked against the NCSM in light systems up to ^{14}C (and up to ^{22}O with the importance-truncated NCSM) [62, 64, 119, 123]. The benchmarks showed that coupled cluster calculations that use a deformed reference state are usually more accurate than those that use a spherical reference.

In contrast to the NCSM, IM-GCM, VS-IMSR, and CC theory, QMC approaches do not rely on a single-particle basis expansion. Variational Monte Carlo (VMC) approximates the solution of the many-body problem by an accurate trial wave function Ψ_T, obtained by applying two- and three-body correlation operators to a Slater determinant of A single-particle wave functions [124, 125]. The optimal set of variational parameters defining the trial wave function is obtained by minimizing the energy expectation value $\langle\Psi_T|H|\Psi_T\rangle$ with dedicated optimization algorithms [126]. The limitations of the variational ansatz are overcome by the Green's function Monte Carlo (GFMC) method that propagates the trial wave function in imaginary-time to extract the ground state of the system $|\Psi_0\rangle = \lim_{\tau\to\infty}|\Psi(\tau)\rangle = \lim_{\tau\to\infty}\exp[-(H - E_0)\tau]\,|\Psi_T\rangle$. QMC methods have no difficulty in using 'stiff' forces that can generate wave functions with high-momentum components, but they are limited to local (or nearly local) Hamiltonians because non-localities exacerbate the fermion-sign problem [127]. There have been QMC studies of the $0\nu\beta\beta$-decay nuclear matrix elements for light nuclei (see, e.g. [128, 129]), but the (nearly) local Hamiltonians [130–134] used in these studies pose a substantial hurdle for direct benchmarks against the configuration-space methods that we discussed above. More recently developed local chiral interactions with typical cutoffs around $\Lambda = 500$ MeV lead to much slower convergence than their nonlocal counterparts with the same scales. Renormalization group transformations may help to mitigate this problem, but the uncertainties due to the omission of induced contributions to the interaction and transition operators may also be more substantial than in a nonlocal regularization scheme. Nevertheless, once RG and EFT truncation errors have been propagated to the $0\nu\beta\beta$ matrix element, a comparison of QMC and configuration-space methods will represent an important check.

3.2.5. Other ab initio approaches. We have focused on the several *ab initio* methods that have already been applied to experimentally relevant transitions, but there are others that may also be able to tackle these nuclei soon. Applications of QMC have been limited almost entirely to the *p*-shell and below because the number of spin/isospin states scale exponentially with particle number A (see, e.g. [135] and references therein). However, within the auxiliary field diffusion Monte Carlo (AFDMC) approach [136] the spin-isospin degrees of freedom are described by single-particle spinors, the amplitudes of which are sampled with Monte Carlo techniques based on the Hubbard–Stratonovich transformation. The transformation reduces the computational scaling from exponential to polynomial in A. AFDMC calculations for ^{16}O have been reported [132], and calculations of ^{48}Ca are conceivable in the near future.

A recently proposed alternative is to use QMC to compute $M_{0\nu}$ for light nuclei, and match an effective shell-model operator to these calculations [61], using the generalized contact formalism (GCF). The effective operator is then employed in shell-model calculations of heavier nuclei, where QMC is not feasible. This approach can be viewed as the QMC providing synthetic data to which a shell-model effective operator can be fit. It is justified by the factorization of physics at the scale of nucleon-nucleon interactions from the nuclear environment. This factorization is seen in the application of renormalization group (RG) methods to QMC wave functions, where short-distance physics in those wave functions evolves into effective operators at the lower resolution appropriate to the shell model [137]. The GCF implements the leading order consequences of factorization. One challenge for the future will be quantifying the long-range correlations missed by the shell model; these will in general depend on the valence space (see effective charges for $E2$ transitions as an example). Such quantification is one aspect of a more general question about what the sub-leading corrections to the GCF calculation carried out in [61] are.

The RG approach to this problem makes it clear that, in *any* of the approaches to the nuclear many-body problem described here, the $0\nu\beta\beta$ operator must be evolved consistently with the methods used to reduce the effective size of the space in which the many-body wave functions are computed. It follows that the $0\nu\beta\beta$ contact operator will not necessarily be the same as the one computed in [79], or obtained in the future from LQCD. Instead, that short-distance operator must absorb the physics between the hadronic scale of LQCD/sum-rule calculations and the low-energy nuclear-structure scale; i.e. it will account not just for hadronic excitations that have been integrated out of the Hilbert space, but for high-momentum nuclear correlations that are integrated out too.

The NCSM may also be applied to heavier isotopes in the future. Although the method in its original form is typically limited to $A \lesssim 16$, the importance-truncated NCSM (IT-NCSM) [138] can significantly reduce the dimensions of the Hamiltonian and thus reach higher in mass, conceivably up to ^{48}Ca. One challenge will be to obtain a better understanding of the extrapolation of $M_{0\nu}$ in the importance truncation parameter $\kappa_{\min}$.

The symmetry-adapted no-core–shell model (SA-NCSM) is a version of the NCSM that uses irreducible representations of the symplectic symmetry group $Sp(3,\mathbb{R})$ rather than particle-hole energy to truncate its basis [139–142]. The alternative truncation scheme allows it to efficiently capture deformation, which is important in either the mother or daughter nucleus in all experimentally relevant $0\nu\beta\beta$-decay candidates. Applications of the SA-NCSM have mostly focused on *p*- and *sd*–shell nuclei so far, but the first results for ^{48}Ti have been reported in [141]. These particular results serve as a demonstration that convergence of a SA-NCSM calculation is mainly affected by the strength of the mixing between irreps in a particular nucleus rather than the mass number: the model space dimension for ^{48}Ti is more than an order of magnitude smaller than the dimension for ^{20}Ne. At present three-nucleon

forces have not yet been included in the SA-NCSM, but once this challenge is overcome, the SA-NCSM will be a valuable complementary approach to the coupled cluster and VS-IMSRG methods that employ particle-hole based truncations. It is also complementary to the IM-GCM because the $Sp(3, \mathbb{R})$ irreps offer a more systematic approach to basis construction than the selection of relevant generator coordinates.

Both the conventional NCSM and SA-NCSM can also be combined with an (MR-) IMSRG preprocessing of the Hamiltonian and transition operators to accelerate convergence [120]. A combination of MR-IMSRG evolution and SA-NCSM, in particular, would embrace a similar philosophy as does the IM-GCM.

3.2.6. Other methods. Besides the *ab initio* methods described in the previous subsections, a variety of other methods have been used to compute $M_{0\nu}$ in nuclei of interest to experimentalists. These others can be broadly grouped into categories: the interacting shell model [143–151], energy-density-functional (EDF) methods [152], the quasi-particle random phase approximation (QRPA) [153–156, 55], and the interacting boson model (IBM) [157, 158].

In this article, the emphasis is on methods that can, in principle, quantify the theoretical uncertainties of the underlying strong-interaction Hamiltonian and of the transition operators. However, methods such as the 'phenomenological' shell model still have a valuable role to play, because they preserve underlying nuclear many-body symmetries and thus capture the most relevant degrees of freedom. In addition, the heavy work of finding optimized effective shell-model Hamiltonians and effective transition operators that capture the landscape of realistic nuclear spectra and of the experimentally accessible nuclear observables has already been done in these approaches. We envision that semi-phenomenological methods, such as the shell model, can be used to explore correlations between observables, helping us identify the quantities that best reflect the accuracy of an *ab initio* calculation. For example, an ensemble of shell model Hamiltonians can be generated by adding random contributions to the two-body matrix elements of some 'seed' Hamiltonians [159]. These Hamiltonians can then be used to obtain $M_{0\nu}$, as well as excitation spectra and electroweak transitions and moments (for which data exist or could be obtained). Any observables which are significantly correlated with $M_{0\nu}$ would then be explored in the more expensive *ab initio* calculations, producing input for subsequent model mixing analysis. An initial study along these lines for the $0\nu\beta\beta$ decay of ^{48}Ca-^{48}Sc-^{48}Ti system can be found in [160]. See also [161].

4. A program for uncertainty quantification

The preceding sections outlined a variety of many-body methods that can be used to perform *ab initio* calculations of $0\nu\beta\beta$ nuclear matrix elements. It might be supposed that the goal of a UQ analysis should be to determine the 'best' of these methods and that whichever method turns out to be 'best' should then be used exclusively. In fact, these methods have complementary strengths and deficiencies, so the goal instead is to use all of them to optimize the overall predictions. Therefore in this section, we outline a procedure, depicted in figure 3, by which the results for $M_{0\nu}$ obtained in those different methods—as well as their uncertainties—can be combined into a single, unified prediction for $M_{0\nu}$. We also explain how that procedure will naturally suggest alternative strategies for calibration of the *ab initio* calculations which should, in turn, lead to refined predictions for $M_{0\nu}$.

Throughout this section, we have in mind that we are considering *ab initio* predictions for $M_{0\nu}$ that are obtained with chiral-EFT forces and decay operators. Differences between

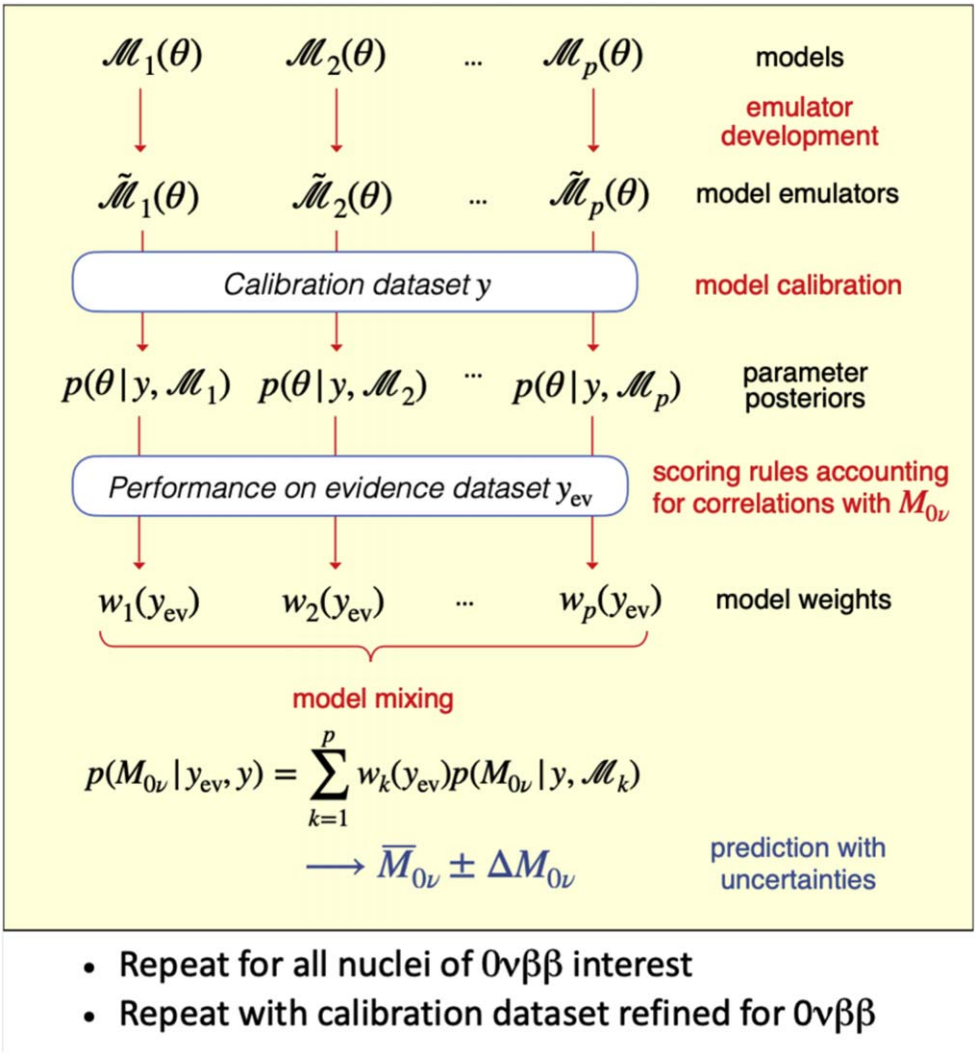

Figure 3. The road to calculations of $M_{0\nu}$ with UQ that accounts for all limitations of the nuclear-physics calculation: truncation errors in chiral-EFT, uncertainties in the theory's parameters, and deficiencies of the many-body methods used. Emulator development is the first step, as it is key to facilitating subsequent calculations. Model parameters θ can be calibrated against a dataset y. Weights for the different many-body methods will be obtained by assessing methods' performance on a set of observables $\{y_{ev}\}$. The weights $w_k(y_{ev})$ are to be computed via scoring rules that gauge predictive accuracy [162] and will also take account of the extent to which different members of $\{y_{ev}\}$ are correlated with $M_{0\nu}$.

different implementations of the chiral-EFT force should therefore be encompassed within the uncertainty assigned due to truncation of the EFT expansion, cf section 2.1 above. The source of uncertainty that is hardest to assess is therefore that due to the use of different methods for solving the A-body problem: these are associated with different ways of truncating the A-body Hilbert space. In what follows we denote the different many-body methods that have been, or may in the future be, adopted to solve this problem as $\mathcal{M}_k$. We treat these as different

'models' in the statistical sense of the term 'model' and seek to combine their predictions into a single prediction that accurately assesses uncertainties in the evaluation of $M_{0\nu}$. We assume that uncertainties due to the truncation of the chiral-EFT expansion are reflected in the posterior distribution that must be provided by each many-body method, $\mathcal{M}_k$.

Method $\mathcal{M}_k$'s prediction also has an inherent parametric uncertainty, coming both from the parameters of the Hamiltonian used to obtain the wave function of the initial and final state in the double-beta-decay process, and from the contact piece of the $0\nu\beta\beta$ operator. In what follows we denote the low-energy constant that multiplies the contact piece by η and the parameters of the Hamiltonian as θ.

Recently, η has been determined [163] by reproducing the synthetic datum, $y_{\rm synth}$ provided in [44, 45]. Meanwhile, for most of this section we will assume that the parameters θ are calibrated to a dataset y (see section 2.2) that does not have to include observables that we expect are correlated with $0\nu\beta\beta$ decay. This is, after all, the stated orientation of most *ab initio* approaches, which calibrate the parameters of *NN* and three-nucleon forces (3NFs) to *NN* scattering data and a few observables in light nuclei. The posterior probability distribution for the parameters θ that is obtained from such an analysis is denoted $p(\theta|y)$.

From a Bayesian perspective, each many-body method's prediction of $M_{0\nu}$ also comes with a systematic error that depends on parameters of the approach employed, e.g. Hilbert space size, accuracy of treatment of 3NFs, etc. The statistical modeling of this systematic error is referred to as discrepancy learning (see equation (2)). Simultaneous learning of discrepancy and parameters is a complicated practical and theoretical exercise. Moreover, with no information to leverage near the quantity of interest $M_{0\nu}$, verification of discrepancy can be difficult. Nonetheless, grounded, informed priors on the discrepancy can improve prediction—especially when we seek to leverage the predictions made across several many-body methods. We therefore write:

$$M_{0\nu}(\text{true}) = M_{0\nu}^{\mathcal{M}}(\theta,\, \eta;\, \lambda) + \delta M_{0\nu}^{\mathcal{M}}(\lambda), \tag{4}$$

where $M_{0\nu}^{\mathcal{M}}(\theta,\, \eta;\, \lambda)$ is the prediction obtained in method $\mathcal{M}$ with method hyperparameters λ (and at specific Hamiltonian and operator parameter values) and $\delta M_{0\nu}^{\mathcal{M}}(\lambda)$ is the corresponding model uncertainty.

If we, for the moment, ignore the issue of the discrepancy function, then the method-$\mathcal{M}$ prediction of $M_{0\nu}$ is formed by marginalizing over θ and η using the distributions established for them from the data $\{y,\, y_{\rm synth}\}$:

$$p(M_{0\nu}|\mathcal{M}) = \int p(M_{0\nu}|\theta,\, \mathcal{M}) p(\theta|y,\, \mathcal{M}) p(\eta|y_{\rm synth},\, \mathcal{M}) \mathrm{d}\theta \mathrm{d}\eta. \tag{5}$$

Here it should be noted that we have allowed for the possibility that the probability density obtained for both the Hamiltonian parameters and η is different for different methods, i.e. depends on the method $\mathcal{M}$. We have, however, assumed that all methods are calibrated using a common dataset y.

But the problem of model discrepancy is critical in predictions for neutrinoless double-beta decay: different approaches to the nuclear many-body problem are based on different physics assumptions, and so have different model discrepancies. In order to get a handle on the model discrepancy we propose to assess that method's ability to predict observables that may share similar physics features to the $0\nu\beta\beta$ decay in the nucleus of interest. Candidate processes include:

- Single β-decay rates in neighboring nuclei, e.g. in the intermediate nucleus in $0\nu\beta\beta$ decay;
- β-strength distributions;

- Known $2\nu\beta\beta$ decay rates [161, 164];
- Magnetic moments and $B(M1)$ rates in the three nuclei involved in any particular $0\nu\beta\beta$ decay;
- Energies of the lowest $J^\pi = 2^+$ states and $B(E2, 2^+ \to 0^+)$ rates in initial and final nuclei;
- Charge radii;
- Observables probing a 100 MeV momentum-transfer scale, e.g. in muon capture.

The idea is then that a method that performs well on these observables, which we denote collectively as $y_{\rm ev}$, should be a more accurate predictor of $M_{0\nu}$ than one that does not.

But which of these observables are most important for constraining the $0\nu\beta\beta$ decay rates? Until now discussion on this point has been largely driven by qualitiative arguments. We propose that, by using properly calibrated Hamiltonians, this question can be answered by analyzing the correlations between the observables on the list above and $M_{0\nu}$. Those correlations can be well approximated by drawing a finite number of samples from $p(\theta|y)$ (say $\approx$100), using one model $\mathcal{M}$ to compute each observable in the set y_{ev} and $M_{0\nu}$, and extracting the empirical correlation coefficient of $M_{0\nu}$ and each quantity in y_{ev} for that model $\mathcal{M}$. Examples of such sensitivity studies can be found in, e.g. [165–167].

A few supplementary points regarding this correlation analysis need to be made:

- This correlation need not be the same in every method. Different methods have different discrepancy functions, because different methods truncate the nuclear many-body problem in different ways. A particular example of this is that methods with different resolution scales may differ in whether their discrepancy function reflects errors in the long-distance physics or errors in the short-distance physics. Indeed, the balance between these two types of errors could shift within a particular method as the value of the hyperparameters λ changes. It follows that the correlation found for method $\mathcal{M}$ at particular values of λ may depend on either λ or $\mathcal{M}$. But, analysis of these correlations, when combined with data on the observables in the set y_{ev}, will help us pin down the discrepancy functions, or at least minimize their impact on the $M_{0\nu}$ prediction.
- The prediction of the observables y_{ev} may depend on additional parameters γ, that are not part of the set θ, and are not *a priori* needed to predict $M_{0\nu}$. The posterior prediction for y_{ev} is then formed by marginalizing over γ, using a probability distribution function that can be thought of as a prior for our purposes, but may be informed by studies of the pertinent observable(s) in nuclei that are some distance from the $0\nu\beta\beta$ candidate

$$p(y_{ev}|y, \mathcal{M}) = \int p(y_{ev}, \theta, \gamma, \mathcal{M}) p(\theta|y) p(\gamma|\mathcal{M}) \mathrm{d}\theta \mathrm{d}\gamma. \tag{6}$$

  Marginalizing over η will certainly be necessary for the prediction of $M_{0\nu}$. Such marginalization (over η and γ) may affect the correlation.

- As discussed in section 3.2.6, the correlation analysis does not need to be initiated within computationally-expensive *ab initio* calculations. In the first instance, it can be carried out using lower resolution approaches that can be viewed as computationally less expensive emulators of *ab initio* methods. Examples of ongoing work along these lines can be found in, e.g. [160, 161, 168, 169].

Such a correlation analysis is useful in its own right. But, with these correlation coefficients in hand we can form an 'improved Bayesian model average' of the results from the different many-body methods $\mathcal{M}$. In BMA [76], a set of candidate methods $\mathcal{M}_1,\ldots,\mathcal{M}_p$ are combined to form a predictive distribution via equation (3):

$$p(M_{0\nu}|y_{ev},\, y) = \sum_{k=1}^{p} w_k(y_{ev}) p(M_{0\nu}|y,\, \mathcal{M}_k), \tag{7}$$

where $w_k(y_{ev})$ represents the underlying weight given to each method. The weight w_k is proportional to $p(y_{ev}|\mathcal{M}_k) \times p(\mathcal{M}_k)$, where $p(y_{ev}|\mathcal{M}_k)$ represents the evidence for method $\mathcal{M}_k$ present in data y_{ev} and $p(\mathcal{M}_k)$ is a prior probability that method k is correct. This prior is usually taken to be flat across the methods $\mathcal{M}_k$, i.e. the methods are all taken to be equally plausible. The formula (7) is aspirational in that there are complications in its deployment that are both practical and theoretical.

The selection of the weights requires careful documentation of the source of the systematic errors between method predictions and observables. Extraneous observables, i.e. observables that are no more than weakly related to $0\nu\beta\beta$, are less dangerous to the resulting inference if all error sources were only experimental and independent throughout the observable space as no method has a specific advantageous bias. However, in the context of $0\nu\beta\beta$ one expects that a significant portion of the error can be attributed to systematic method deficiencies $\delta y_{\rm th}$. The result is significantly related error that exists across the observable space.

It is therefore critical to carefully select observables in y_{ev}. Observables that are closely related to the target observable, $y^* = M_{0\nu}$ should receive higher weights—something that classical BMA does not do. If observables in y_{ev} that are not significantly related to $M_{0\nu}$ can influence the weight of a method in the BMA formula (7), they are likely to dilute—or even bias—the prediction for $M_{0\nu}$. Parsimony is also important for a practical reason: the Bayesian model averaging formula requires the same y_{ev} should be used across all many-body methods, meaning all of them need to be able to produce predictions of these quantities. A parsimonious choice of observables makes it more feasible that y_{ev} can be predicted in all candidate approaches to the nuclear many-body problem.

The program for UQ that we have laid out up to this point in the section could be carried out using *ab initio* methods and already calibrated chiral-EFT forces and operators. We now discuss a longer-term strategy for refining the prediction of $M_{0\nu}$. Once it has been established which observables in y_{ev} are strongly correlated with $M_{0\nu}$ the predictive power of the methods $\mathcal{M}_k$ can be improved by including those members of the dataset y_{ev} in the dataset used to calibrate the nuclear Hamiltonian and decay operators. The parameter vector θ would then be readjusted within each calculation $\mathcal{M}_k$. This would open a window for a more refined combined prediction of the different many-body methods.

One critical challenge to overcome is providing predictions of quantities for various values of θ, η, and γ for all methods. Part of this is needed for the integration to compute $p(y|\mathcal{M}_k)$—see equations (5) and (6)—where MCMC must be leveraged for both the core Hamiltonian parameters θ as well as the ancillary parameters γ and the $0\nu\beta\beta$ parameter η. This problem is amplified in the case of high-dimensional parameter space.

There are a few statistical and computational tools that can be deployed to resolve this problem. Firstly, reducing the space of parameters through screening will be critical for each method, thereby including only the parameters that are critical for predicting y_{ev} and $M_{0\nu}$. Secondly, emulators (or surrogates) can play a vital role to conduct Bayesian inference from only a few full *ab initio* evaluations of the matrix element. Emulators can take on a variety of forms but the function is shared: to provide a computationally inexpensive approximation of y_{ev} and $M_{0\nu}$ for any value of θ, η, and γ. Gaussian process-type emulators exploit smoothness in the computation's response to the parameters. Other reduced-basis emulators instead build modified, cheaper alternatives to the full *ab initio* result when it is subject to specific structure [170–175]. Variational machine learning methods [176–178] form another path that produce efficient emulators that intrinsically learn the optimal latent parameter space needed for robust

interpolation and prediction. These methods have an advantage over many forms of emulation as they can learn highly non-linear manifolds while still generating a notion of the emulators' internal uncertainty.

One common theme across all methods is they rely on using specific computations at designated parameter combinations to build predictions at other ones. The amount of computations needed to build an adequate emulator varies across methodologies. Classical literature on Gaussian process-type emulators suggest computing at ten times the dimension of the parameters, but that suggestion has recently been reconsidered and higher-dimensional parameter spaces perhaps need more computation. Good emulators will naturally come with their own uncertainty quantification, which is critical for producing valid approximations of $p(y_{ev}|\mathcal{M}_k)$ as well as predictions of $p(M_{0\nu}|\mathcal{M}_k)$.

As mentioned above, lower resolution approaches, such as DFT, can be used to construct emulators of higher resolution *ab initio* methods. This construction can follow equation (2) in which $y_{\rm exp}(x;\,\theta)$ is replaced by *ab initio* predictions and the model discrepancy $\delta y_{\rm th}$ would model the difference between predictions of *ab initio* and lower resolution models.

5. Summary

Accurate calculation of the nuclear matrix elements governing neutrinoless double-beta decay, with quantified uncertainty, is essential for the success of the impressive experimental and theoretical worldwide effort in this area [37]. The purpose of this article is to lay out the challenges to the nuclear-theory community—in regard to both nuclear-physics calculations and uncertainty quantification therein—and map out a path for near- and long-term progress.

It will require a concerted effort in both LQCD and EFT, as well as the coupling of these theories, to fully quantify the theoretical uncertainties related to the $0\nu\beta\beta$-decay operator and associated matrix elements at the hadronic level. Systematic improvements in nuclear many-body methods are underway, and should be ready to produce a new generation of $M_{0\nu}$ matrix elements in the next few years. The complexity of the problem makes the use of multiple many-body methods well worthwhile. Their complementary strengths and deficiencies cannot only be exploited for validation but also combined through Bayesian methods to yield better overall predictions.

The implementation and application of both QCD/chiral-EFT and nuclear many-body approaches will require exascale computing resources and beyond. One focus of future work in this area will be ensuring optimal use of the heterogeneous architectures that characterize leadership-class computers.

A crucial feature of our paper is the emphasis it places on UQ. Without principled UQ, the usefulness of predicted $M_{0\nu}$ values for guiding experimental efforts, interpreting measurements, and assessing new physics will be limited. At present, few physicists working on the problem of $M_{0\nu}$ make informed choices about UQ, understand the modern UQ glossary, or consider UQ to be an essential part of 'the answer'. This situation can be improved through coherent inter-disciplinary collaboration of nuclear physicists with applied mathematicians, statisticians, and computer-science experts.

Such a collaboration could carry out the concrete, multi-staged, and interwoven program of nuclear-physics and UQ methodological improvements and computations laid out in this article. In concert with continued strong support for the efforts of PIs and research groups working on $0\nu\beta\beta$ decay, this will make the ultimate goal of accurate and precise $M_{0\nu}$ predictions achievable.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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