Ab Initio Uncertainty Quantification of Neutrinoless Double-Beta Decay in ^{76}Ge

A. Belley,[1,2,*] J. M. Yao (尧江明),[3,†] B. Bally,[4] J. Pitcher,[1,2] J. Engel,[5] H. Hergert,[6,7] J. D. Holt,[1,8] T. Miyagi,[9,10,11] T. R. Rodríguez,[12,13,14] A. M. Romero,[15,16] S. R. Stroberg,[17] and X. Zhang (张馨)[3]

[1]*TRIUMF, Vancouver, British Columbia, Canada*
[2]*Department of Physics & Astronomy, University of British Columbia, Vancouver, British Columbia, Canada*
[3]*School of Physics and Astronomy, Sun Yat-sen University, Zhuhai 519082, People's Republic of China*
[4]*ESNT, IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*
[5]*Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27516-3255, USA*
[6]*Facility for Rare Isotope Beams, Michigan State University, East Lansing, Michigan 48824-1321, USA*
[7]*Department of Physics & Astronomy, Michigan State University, East Lansing, Michigan 48824-1321, USA*
[8]*Department of Physics, McGill University, Montréal, Quebec, Canada*
[9]*Technische Universität Darmstadt, Department of Physics, 64289 Darmstadt, Germany*
[10]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
[11]*Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[12]*Departamento de Estructura de la Materia, Física Térmica y Electrónica, Universidad Complutense de Madrid, E-28040 Madrid, Spain*
[13]*Departamento de Física Teórica, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[14]*Centro de Investigación Avanzada en Física Fundamental-CIAFF-UAM, E-28049 Madrid, Spain*
[15]*Departament de Física Quàntica i Astrofísica (FQA), Universitat de Barcelona (UB), c. Martí i Franqués, 1, 08028 Barcelona, Spain*
[16]*Institut de Ciències del Cosmos (ICCUB), Universitat de Barcelona (UB), c. Martí i Franqués, 1, 08028 Barcelona, Spain*
[17]*Department of Physics and Astronomy, University of Notre Dame, Notre Dame, Indiana 46556, USA*

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The observation of neutrinoless double-beta ($0\nu\beta\beta$) decay would offer proof of lepton number violation, demonstrating that neutrinos are Majorana particles, while also helping us understand why there is more matter than antimatter in the Universe. If the decay is driven by the exchange of the three known light neutrinos, a discovery would, in addition, link the observed decay rate to the neutrino mass scale through a theoretical quantity known as the nuclear matrix element (NME). Accurate values of the NMEs for all nuclei considered for use in $0\nu\beta\beta$ experiments are therefore crucial for designing and interpreting those experiments. Here, we report the first comprehensive *ab initio* uncertainty quantification of the $0\nu\beta\beta$-decay NME, in the key nucleus ^{76}Ge. Our method employs nuclear strong and weak interactions derived within chiral effective field theory and recently developed many-body emulators. Our result, with a conservative treatment of uncertainty, is an NME of $2.60^{+1.28}_{-1.36}$, which, together with the best-existing half-life sensitivity and phase-space factor, sets an upper limit for effective neutrino mass of 187^{+205}_{-62} meV. The result is important for designing next-generation germanium detectors aiming to cover the entire inverted hierarchy region of neutrino masses.

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Introduction.—The origin of the matter-antimatter asymmetry in the Universe remains one of the most important unsolved puzzles in physics. Many theories suggest that the asymmetry originates from a violation of lepton number through *leptogenesis* [1], in which leptons are created with no corresponding antileptons. The most promising way at present to determine the level at which lepton number is violated is through the hypothetical nuclear transition known as neutrinoless double-beta ($0\nu\beta\beta$) decay [2], in which two neutrons inside an atomic nucleus are transmuted into two protons, and two electrons are emitted without any of the antineutrinos that lepton-number conservation requires. The detection of $0\nu\beta\beta$ decay would immediately demonstrate that neutrinos are Majorana fermions [3], i.e., their own antiparticles, and therefore have significant implications for the Universe's matter-antimatter asymmetry. Furthermore, if $0\nu\beta\beta$ decay is mediated by light Majorana neutrino exchange, its half-life can be related to an effective neutrino mass $\langle m_{\beta\beta}\rangle = \sum_i U_{ei}^2 m_i$, where m_i are the masses of light neutrinos, and U_{ei} are elements of the unitary matrix that mixes electron neutrinos with other flavors. The precision with which $\langle m_{\beta\beta}\rangle$ can be determined depends on how well the nuclear matrix element (NME) that governs the decay can be calculated.

^{76}Ge is one of only a few highly promising candidate nuclei for experiments, as germanium detectors possess the advantages of high energy resolution, low internal background, and high detection efficiency. Several experiments have been searching for $0\nu\beta\beta$ decay in this isotope, including the GERDA [4], Majorana Demonstrator [5], and CDEX [6] collaborations. The highest half-life sensitivity so far has been reported by the GERDA experiment, which set a limit $T_{1/2} > 1.8 \times 10^{26}$ years at 90% confidence level (C.L.) [4]. If light-neutrino exchange is responsible, this half-life limit establishes an upper limit for the effective neutrino mass of $\langle m_{\beta\beta}\rangle = 73$–204 meV. The large range is due mainly to a spread of about a factor of 3 in the NMEs predicted by different nuclear models [7–13]. The spread can be even larger when the NMEs from all existing calculations with different parametrizations are considered. The associated uncertainty is difficult to reduce because each model has its particular phenomenological assumptions and uncontrolled approximations [14–17].

In recent years, significant progress has been made in calculating NMEs from first principles. The required advances in *ab initio* nuclear theory have followed the parallel development of nuclear forces from chiral effective field theory (χEFT) [18,19], a systematically improvable low-energy expansion of QCD, where undetermined low-energy constants (LECs) are optimized to data in few-nucleon systems, and similarity-renormalization-group (SRG) methods [20] for evolving such forces to the low-energy scale typical for atomic nuclei. With the resulting interactions and operators, the A-body Schrödinger equation can now be solved fairly accurately for most atomic nuclei in the medium-mass region [21], and even in the ^{208}Pb region [22], by employing nonperturbative and systematically improvable many-body methods. The application of *ab initio* methods to $0\nu\beta\beta$ decay is important because theoretical uncertainties related to the many-body wave functions and transition operators become controllable.

Advances in the development of *ab initio* methods have enabled a first wave of multimethod calculations of NMEs for $0\nu\beta\beta$ decay in a set of light nuclei using different chiral nuclear forces [23–25]. In particular, three *ab initio* methods, the in-medium generator coordinate method (IM-GCM) [26], the valence-space formulation of the in-medium SRG (VS-IMSRG) [27], and coupled-cluster theory [28], have been used to calculate the NME of ^{48}Ca, the lightest nucleus that could be used in an experiment. When starting from the same chiral two-nucleon-plus-three-nucleon (NN + 3N) interaction and $0\nu\beta\beta$-decay operators, the approaches obtain results that agree within roughly estimated uncertainties. These methods were also successfully benchmarked against one another, as well as against quasiexact diagonalization in light nuclei [24,25,28]. The difference between NMEs for $0\nu\beta\beta$ decay calculated with different *ab initio* methods but the same input has been found to give a useful approximation to the inaccuracies caused by truncation in many-body methods. These studies make it feasible to carry out uncertainty quantification in the *ab initio* prediction of the NMEs of experimentally relevant nuclei.

The second-lightest such nucleus, ^{76}Ge, is, along with ^{136}Xe, one of the two most important isotopes for experimental searches, and is now within the reach of multiple *ab initio* methods. The VS-IMSRG was the first *ab initio* approach to calculate the NME for ^{76}Ge, using the long-range (LR) transition operator associated with standard light-neutrino exchange [27]. The resulting NME, 2.14(9), was 25%–45% smaller than those obtained from phenomenological shell-model calculations. However, the contributions of the recently discovered leading-order (LO) short-range (SR) contact transition operator [29] and higher-order terms were not evaluated. In this work, we now include these contributions. In particular, we report the results from the IM-GCM calculation and present the first comprehensive uncertainty quantification for the NME in ^{76}Ge using strong and weak interactions consistently derived within χEFT.

Quantifying the uncertainty in the $0\nu\beta\beta$-decay NME.—For the $0\nu\beta\beta$ decay $^{76}\mathrm{Ge}(0_1^+) \to {}^{76}\mathrm{Se}(0_1^+) + 2e^-$, the NME, called $M^{0\nu}$, can be written as

$$M^{0\nu} = \langle {}^{76}\mathrm{Se}(0_1^+)|\hat{O}^{0\nu}|{}^{76}\mathrm{Ge}(0_1^+)\rangle, \quad (1)$$

where the decay operator $\hat{O}^{0\nu}$ is derived in the standard mechanism, depicted in Fig. 1(a). The wave functions are obtained with the two *ab initio* methods, i.e., IM-GCM and VS-IMSRG. The main challenge in the assessment of theoretical error is the propagation of the uncertainties in the LECs from the chiral interaction through the complicated many-body calculations that ultimately produce the NME. To this end, we use the sampling and importance resampling [30] formulation of Bayes's theorem for discrete samples, as was done in Ref. [22] to obtain a theoretical uncertainty on the neutron skin of ^{208}Pb.

Following this procedure, *a posterior* predictive distribution (PPD) of the NMEs depending on the LECs ($\mathbf{c}$) is given by

$$\mathrm{PPD} = \{M_k^{0\nu}(\mathbf{c})\colon\ \mathbf{c} \sim \mathcal{P}(\mathbf{c}|\mathrm{calibration})\}, \quad (2)$$

where $M_k^{0\nu}$ represents the NME from a specific theoretical calculation (i.e., using a particular many-body method and operators truncated at order k) and $\mathcal{P}(\mathbf{c}|\mathrm{calibration})$ represents the probability of an LEC sample to yield results for a set of calibration observables that match experimental data. We label the standard deviation coming from this (non-Gaussian) distribution ϵ_{LEC} to make comparison with other sources of error easier. As calibration observables, we use properties of nuclei of mass $A = 2$–4 and $A = 16$ as done in Ref. [32] to which we add the neutron-proton scattering phase shift in the $^1S_0$ partial wave at lab energy of 50 MeV, since it has recently been discovered to correlate strongly with the NMEs [33]. The NMEs for the LEC samples are then evaluated using the recently developed

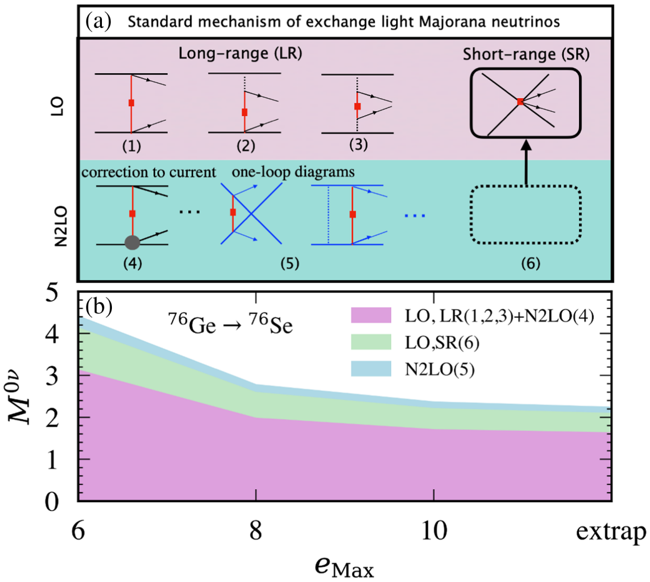

FIG. 1. Hierarchy of contributions to $0\nu\beta\beta$ decay in chiral EFT, assuming light Majorana neutrino exchange. (a) Diagrammatic contributions at different orders. A short-range contribution is promoted from N2LO to LO in order to ensure renormalizability, as indicated by the arrow. (b) The convergence of the NMEs for ^{76}Ge → ^{76}Se using LO and N2LO transition operators. The red square indicates an insertion of Majorana neutrino mass term $\langle m_{\beta\beta}\rangle$, and the gray circle represents corrections to the single-nucleon current parametrized in terms of form factors. The results are obtained from IM-GCM calculations using the EM1.8/2.0 chiral NN + 3N interaction [31] as a function of $e_{\rm Max}$.

multioutput multifidelity deep Gaussian process (MM-DGP) emulator [34] for the VS-IMSRG, which allows us to, within minutes, predict the results of billions of many-body calculations that would otherwise take years to perform in full. The error $\epsilon_{\rm LEC}$ could be reduced by going to a higher order in the chiral truncation, allowing for a better match with multiple calibrating observables due to the inclusion of more parameters. Alternatively, identifying additional nuclear observables that are strongly correlated with the NMEs and incorporating them into the calibrating observables could further refine the distribution.

We further assume that our errors are normally distributed and mutually independent, such that the true value of the NME in Eq. (1) can be written as

$$M^{0\nu} = M^{0\nu}_k + \epsilon_{\chi\rm EFT} + \epsilon_{\rm MBT} + \epsilon_{\rm OP} + \epsilon_{\rm EM}, \qquad (3)$$

where $\epsilon_{\chi\rm EFT}$ represents the error coming from truncation of the nuclear forces, $\epsilon_{\rm MBT}$ the error from the many-body method, $\epsilon_{\rm OP}$ the error due to the truncation of the decay operator, and finally, $\epsilon_{\rm EM}$ the error on the emulated results. The values of the NME, together with the errors ϵ_i from different sources, are presented in Table I. We detail below how each uncertainty is assessed.

TABLE I. The recommended value for the total NME of $0\nu\beta\beta$ decay in ^{76}Ge, together with the uncertainties from different sources.

$M^{0\nu}$	$\epsilon_{\rm LEC}$	$\epsilon_{\chi\rm EFT}$	$\epsilon_{\rm MBT}$	$\epsilon_{\rm OP}$	$\epsilon_{\rm EM}$
$2.60^{+1.28}_{-1.36}$	0.75	0.3	0.88	0.47	< 0.06

We employ nuclear interactions derived from χEFT where the Δ isobars are considered explicitly [35]. In particular, these interactions are given at next-to-next-to-leading order (N2LO) in the chiral expansion, where 17 LECs arise. These interactions are particularly useful for the present study since more diagrammatic contributions are considered at a given order in a Δ-full theory than in a Δ-less one, and the LECs come out more natural.

To assess $\epsilon_{\chi\rm EFT}$, we estimate the contributions coming from neglected higher orders using a recently developed technique [36]. By examining the order-by-order NME convergence, we obtain 0.27 (68% C.L.) with the Δ-full interaction [35]. To be conservative, we choose $\epsilon_{\chi\rm EFT}$ to be 0.3, as other parametrizations might have a slower rate of convergence. The results are shown in the Supplemental Material [37], compared to the convergence of particular Δ-less nuclear interactions, available at NLO, N2LO, N3LO, and N4LO [68,69]. As expected, we find more rapid convergence for the Δ-full interaction. Additionally, we observe the change from N3LO to N4LO to be much smaller, indicating that a future analysis with nuclear interactions at N3LO would allow us to greatly reduce that uncertainty.

To estimate $\epsilon_{\rm MBT}$, two *ab initio* methods, i.e., IM-GCM [26] and VS-IMSRG [70] are employed. These calculations are carried out using the chiral interaction EM1.8/2.0 [71], where the previous VS-IMSRG value [27] was found to be $M^{0\nu}_{\rm LR} = 2.14(9)$. Here we also compute the contribution of the SR contact transition operator and find an overall ~40% increase in the NME to $M^{0\nu} = 2.94(8)$, with uncertainty coming from both the single-particle basis extrapolation to infinity as well as reference state dependence. Similar calculations are carried out with the IM-GCM, yielding a long-range NME of $M^{0\nu}_{\rm LR} = 1.67$ and total NME of $M^{0\nu} = 2.13$, including the contributions of diagrams (1-4, 6) in Fig. 1(a). Considering the possible contribution from the extension of the IM-GCM model space with cranking configurations, which turn out to enhance the NME by about 10%, we recommend the value $M^{0\nu} = 2.24(11)$. In both approaches we find that the NMEs are significantly increased by the SR transition operator, confirming that it contributes at LO. On the other hand, the results show a modest deviation, where the VS-IMSRG NME is ~30% larger than that from the IM-GCM. We use the largest discrepancy of 0.88 as an estimate of $\epsilon_{\rm MBT}$, which was shown be a reasonable approximation to the inaccuracies caused by

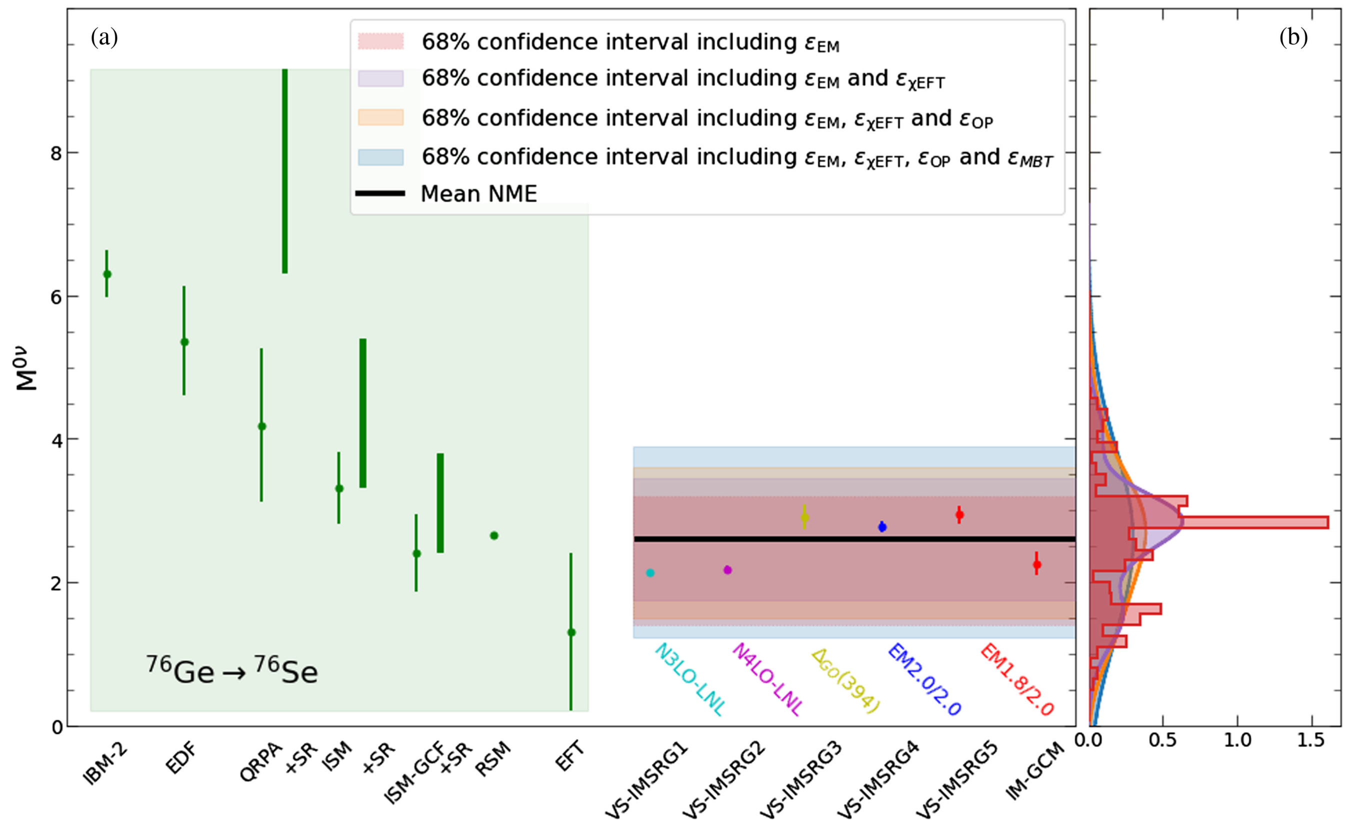

FIG. 2. Comparison of $0\nu\beta\beta$-decay NMEs in ^{76}Ge from nuclear models and *ab initio* calculations. (a) The NMEs from phenomenological models, including the interacting-boson model (IBM-2) [9,62], energy-density-functional (EDF) methods [8,11], quasiparticle random-phase approximation (QRPA) [12,63,64], interacting shell model (ISM) [7,10], ISM with generalized contact formalism (ISM-GCF) [65], realistic shell model (RSM) [13], and EFT [66], are compared to the results of the VS-IMSRG and IM-GCM using different chiral interactions. The error bars of phenomenological nuclear models reflect the discrepancy of calculations from different groups and the bands shows results with the SR contributions included [65,67]. (b) The posterior distribution function of the $0\nu\beta\beta$ NME using the MM-DGP emulator of the VS-IMSRG with 8188 nonimplausible samples of chiral interactions from which the confidence intervals are extracted.

truncation in light nuclei [25]. This difference is somewhat larger than what was found in ^{48}Ca [26,27]. This can be understood from the fact that the low-lying states in ^{48}Ca and ^{48}Ti are relatively simple and the quadrupole collectivity of ^{48}Ti is adequately captured in both methods. In contrast, the low-lying states of ^{76}Ge and ^{76}Se exhibit strong shape coexistence and collectivity, including significant triaxiality [72–74]. While these collective degrees of freedom are difficult to capture within the VS-IMSRG and other *ab initio* methods starting from spherical references [75,76], they are efficiently incorporated within the IM-GCM, as can be seen from the predicted excitation spectra and electric multipole transitions [72,73]. We expect that future systematic improvements to the many-body truncations will improve the agreement between the two methods.

The errors ϵ_{OP} from the transition operators can be separated into three sources: the use of the closure approximation for the intermediate odd-odd nucleus, the determination of the LEC of the SR transition operator, and the truncation of contributions beyond LO in the operator expansion. The potential error stemming from the closure approximation has been assessed with phenomenological nuclear models [77,78] to be around 10% of the LR NME. This finding aligns with the expectation that contributions depending on the excitation energies of intermediate states belong to the N2LO [79]. Recent nuclear shell-model calculations [80] of the N2LO corrections to the closure approximation also found that they reduce the matrix elements by ~10%. Eventually, these contributions will need to be tackled explicitly in our methods as well as we improve the precision of our NMEs. Figure 1(a) presents different contribution to the $0\nu\beta\beta$-decay operators at LO and N2LO, noting that there is no contribution at NLO. Figure 1(b) displays the convergence of the NMEs at LO and N2LO with respect to e_{Max}, the number of harmonic oscillator major shells in the basis, in the IM-GCM calculation [37]. The value of the LEC for the SR transition operator is determined by fitting the transition amplitude of $nn \rightarrow ppe^{-}e^{-}$ process following Ref. [81]. The SR transition contribution is found to be $M^{0\nu}_{\rm SR} = [0.399, 0.526]$, where the about 27% uncertainty is propagated from the synthetic datum [82,83]. We note that the subleading nuclear interactions are treated slightly differently in many-body methods from that for the synthetic datum. This difference might impact the extracted value of the coupling constant for the SR term. However, because the error of the NME is presently dominated by that of many-body truncation, we leave the quantification of this minor error for the future. We compute the contribution of the genuine N2LO transition operators, cf. Fig. 1, which cannot be absorbed into the form factors, while excluding the contributions requiring intermediate states of odd-odd nucleus. The correction of transition operators at N2LO to the NME shows a weak dependence on the renormalization scale μ, and is found to be 0.079 at $\mu = 500$ MeV, consistent with previous findings [84]. This confirms that the N2LO contributions are small, and the power counting works well for the transition operators. It also suggests that the common practice of taking LO transition operators supplemented with dipole form factors is a good approximation, once the contact term is properly considered. We note, however, that the $0\nu\beta\beta$ operators we used do not explicitly include Delta isobars while our nuclear interactions do. We are not aware of any prior investigations of their impact on the transition, but we expect corrections to appear at N2LO at the earliest, hence any effects due to this discrepancy should be small. In short, we take a conservative value $\epsilon_{\rm OP} = 0.47$ which includes 0.26 from the use of closure approximation, 0.13 from the uncertainty of the LEC of the SR transition operator, and 0.08 from the truncation on the chiral expansion of transition operators.

Finally, $\epsilon_{\rm EM}$ is given by the MM-DGP emulator based upon Gaussian processes, which inherently come with a variance for each prediction. We obtain the final predictive posterior distribution by sampling the PPD 10^8 times and adding errors independently sampled from a normal distribution for each ϵ term. Figure 2 shows the PPDs obtained with each error term discussed above, added separately. We find that $M^{0\nu} = 2.60^{+1.28}_{-1.36}$, where the uncertainty represents a 68% confidence interval. We compare the PPD with results obtained from the VS-IMSRG and IM-GCM methods, using the EM1.8/2.0 interaction [31] and VS-IMSRG with four other state-of-the-art chiral NN + 3N interactions [31,35,85]. All these fall within our confidence interval. Our predictions are further compared to NMEs from various phenomenological nuclear models, where the contribution of the SR transition operator is usually not considered due to the challenge in determining the corresponding LEC in such approaches. With the LECs's value estimated by considering the charge-independence-breaking coupling of nuclear Hamiltonians, the contribution of the SR operator was quantified with the ISM and QRPA [67]. Taking this into account, the discrepancy among different phenomenological models can exceed one order of magnitude, as depicted in Fig. 2.

Conclusions.—In summary, we have presented the first, to our knowledge, comprehensive uncertainty quantification in *ab initio* calculations of NMEs for the $0\nu\beta\beta$ decay of ^{76}Ge using nuclear interactions derived from χEFT and recently developed many-body emulators based on the standard mechanism of exchanging light Majorana neutrinos with transition operators truncated up to the N2LO. We have demonstrated that the NME converges rapidly with the chiral expansion, both for the transition operators and for the strong interactions. Considering the uncertainties stemming from different selections of chiral interactions and many-body solvers, our recommended value for the NME stands at $2.60^{+1.28}_{-1.36}$ (68% C.L.). This, in conjunction with the best half-life sensitivity of $T_{1/2} > 1.8 \times 10^{26}$ years [4], phase-space factor of $G_{0\nu} = 0.237 \times 10^{14}$ years^{-1} [86,87], and the axial-vector coupling strength $g_A = 1.27$, sets the current upper limit for the effective neutrino mass at 187^{+205}_{-62} meV. It is important to note that the current uncertainty encompasses estimated errors from both operators and many-body solvers, presumed to be mutually independent, serving as a reasonable initial framework. While this uncertainty remains substantial, an effective strategy to mitigate it is now available by considering nuclear interactions that go to higher order in the chiral expansion, reducing many-body truncation errors and improving the likelihood function with a few more relevant observables. With our NME, the next-generation tonne-scale Germanium experiment with the ability to discover $0\nu\beta\beta$ decay up to 1.3×10^{28} years [88] will set the upper limit on effective neutrino mass $\langle m_{\beta\beta}\rangle = 22^{+24}_{-7}$ meV, which encompasses almost the entire range of allowed values of inverted neutrino mass hierarchy. This paper complements recent NME calculations in heavy systems [89], illustrating the power of *ab initio* methods to potentially deliver quantified uncertainties for all key isotopes of experimental interest.

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[*]Co-lead author.

[†]Co-lead author. Corresponding author: yaojm8@sysu.edu.cn

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