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New determination of double-β-decay properties in ^{48}Ca: High-precision $Q_{\beta\beta}$-value measurement and improved nuclear matrix element calculations

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We report a direct measurement of the $Q_{\beta\beta}$ value of the neutrinoless double-β-decay candidate ^{48}Ca at the TITAN Penning-trap mass spectrometer, with the result that $Q_{\beta\beta} = 4267.98(32)$ keV. We measured the masses of both the mother and daughter nuclides, and in the latter case found a 1 keV deviation from the literature value. In addition to the $Q_{\beta\beta}$ value, we also present results of a new calculation of the neutrinoless double-β-decay nuclear matrix element of ^{48}Ca. Using diagrammatic many-body perturbation theory to second order to account for physics outside the valence space, we constructed an effective shell-model double-β-decay operator, which increased the nuclear matrix element by about 75% compared with that produced by the bare operator. The new $Q_{\beta\beta}$ value and matrix element strengthen the case for a ^{48}Ca double-β-decay experiment.

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I. INTRODUCTION

The discovery of neutrino oscillations represents the first evidence for new physics beyond the standard model [1,2]. The oscillations conclusively demonstrate that neutrinos have mass, that flavor eigenstates are mixtures of mass eigenstates, and that neutrino physics is more complicated than we had thought. The observation of neutrinoless double-β ($0\nu\beta\beta$) decay, extremely rare if it exists, would at once fill multiple gaps in our understanding of the neutrino's nature and would represent a major breakthrough for particle physics. Since this lepton-number-violating process can occur only if the neutrino is its own antiparticle, its discovery would unambiguously confirm the neutrino as a Majorana particle, while a measured lifetime would provide a value for the neutrino mass scale [3]. This lifetime is given by

$$\left(T_{1/2}^{0\nu}\right)^{-1} = G_{0\nu}(Q_{\beta\beta},Z)|M_{0\nu}|^2 \frac{\langle m_{\beta\beta}\rangle}{m_e}, \tag{1}$$

where the phase space factor $G_{0\nu}$ depends on the Q value and the nuclear charge Z, $|M_{0\nu}|$ is the nuclear matrix element, $\langle m_{\beta\beta}\rangle$ is the neutrino's effective Majorana mass, and m_e is the electron's mass. For each $0\nu\beta\beta$ candidate, two quantities must be accurately determined: a phase-space factor, which depends on the $Q_{\beta\beta}$ value of the decay, and a nuclear matrix element, which is not observable and therefore must be obtained from nuclear structure theory.

The 12 nuclides that have been observed to undergo two-neutrino double-β ($2\nu\beta\beta$) decay [4,5] are the basis for a number of large-scale experimental $0\nu\beta\beta$-decay searches currently underway. Several factors are considered in designing such experiments, among them the Q value. A large $Q_{\beta\beta}$ value is desirable first to enhance the phase-space factor, which scales roughly as the Q value to the fifth power, and second to discriminate against background. The background from naturally occurring radiation falls off sharply above 2.6 MeV, the γ-ray energy of ^{208}Tl (from the ^{232}Th decay chain). In addition, high precision in the $Q_{\beta\beta}$ value and high detector resolution are required in order to distinguish the $0\nu\beta\beta$-decay peak from the irreducible $2\nu\beta\beta$-decay background. Indeed, for the uncertainty of the $Q_{\beta\beta}$ value to be negligible in the data analysis, the uncertainty must be smaller than the intrinsic detector resolution. Of all $0\nu\beta\beta$ candidates, ^{48}Ca possesses the largest $Q_{\beta\beta}$ value, 4.3 MeV [6], which maximizes the signal-to-noise ratio and substantially increases the $0\nu\beta\beta$-decay rate. This quantity was the subject of a high-precision and high-accuracy measurement at TRIUMF's Ion Trap for Atomic and Nuclear science (TITAN) facility and reported

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herein. As ^{48}Ca suffers the lowest isotopic abundance of any candidate, enrichment is required, and recent technical developments [7] have paved the way for increasingly large experiments.

^{48}Ca has been either studied or under investigation for several scintillator-based experiments [7]. At NEMO-III, it was found that $T_{1/2}^{2\nu} = 4.2^{+2.1}_{-1.0} \times 10^{19}$ yr, while the CANDLES project led to the limit $T_{1/2}^{0\nu} > 5.8 \times 10^{19}$ yr. Now relocated at the Kamioka Underground Observatory, the CANDLES detector uses CaF$_2$ crystals immersed in two liquid scintillators and is expected to have a sensitivity of $T_{1/2}^{0\nu} > 3.7 \times 10^{24}$ yr. Concurrently, efforts are being made to achieve a 2% chemical enrichment for the next-phase, 2-ton detector. With improvements in energy resolution, the expected sensitivity for this detector is $T_{1/2}^{0\nu} > 2.5 \times\ 10^{25}$ yr. More recently, ^{40}Ca^{100}MoO$_4$ crystals (depleted in ^{40}Ca) have been proposed by the AMoRE Collaboration, which is working on ^{100}Mo enrichment. Should the $0\nu\beta\beta$-decay peak be observed at any of these experiments and the half-life measured, the nuclear matrix element is required in order to extract the Majorana mass of the neutrino.

^{48}Ca occupies a unique position among $0\nu\beta\beta$-decay candidates in that its relatively low mass and doubly magic nature make it a near ideal case for several *ab initio* many-body methods developed for medium-mass nuclei. Here, we applied chiral nuclear forces [8] and diagrammatic many-body perturbation theory to calculate an effective shell model $0\nu\beta\beta$-decay operator for ^{48}Ca. We found an increase in the nuclear matrix element of $\approx$75% compared to that produced by the bare operator alone, and estimated a further increase of $\approx$8% from moving beyond the closure approximation. To derive the decay rate, the resulting nuclear matrix element is combined with the newly measured $Q_{\beta\beta}$ value at TITAN.

II. EXPERIMENTAL DETAILS

TITAN is an ion trap system coupled to the TRIUMF Isotope Separation and ACceleration (ISAC) rare beam facility. It consists of three traps: a radiofrequency quadrupole (RFQ) beam cooler and buncher [11], an electron beam ion trap (EBIT) [12], and a measurement Penning trap (MPET) [13]; the EBIT was not used in this experiment. Ions were delivered from either ISAC's off-line ion source (OLIS) [14] or TITAN's surface-ionization ion source (TIS). For the production of ^{48}Ca$^+$, an enriched ion source was heated in the TIS whereas ^{48}Ti$^+$ and ^{14}N^{18}O^{16}O$^+$ ions were produced with OLIS. The beams from the TIS and OLIS were delivered independently.

The continuous beam from either ion source was accumulated, cooled, and bunched in the RFQ. A fast time-of-flight mass filter [15] placed between the RFQ and the MPET and a dynamic capture process in the Penning trap ensured pure isobaric ion bunches in the MPET. In addition, dipole cleaning [16] was applied to remove any remaining contaminant ions. In a Penning trap, the mass of an ion is measured via the determination of the cyclotron frequency $2\pi\nu_c = q/m \times B$, where q/m is the charge-to-mass ratio and B the magnetic field strength. The masses were determined using two excitation schemes: the conventional time-of-flight ion-cyclotron-resonance (TOF-ICR) method [17,18], whereby the ions were excited with a continuous RF field for a time T_{RF} [Fig. 1(a)] and the Ramsey technique [10,19], wherein the oscillatory field was applied in two pulses separated by a waiting period [Fig. 1(b)]. For this, two 200-ms RF pulses were spaced apart by 1553 ms, denoted as 200-1553-200 ms. The ν_c measurements of ^{48}Ca$^+$, ^{48}Ti$^+$, and N^{18}OO$^+$ were interleaved; thus, the primary experimental result is the ratio of their cyclotron frequencies, listed in Table I. A statistical uncertainty of $\delta R/R = 3 \times 10^{-9}$ was achieved. Systematic uncertainties were carefully evaluated. These include simultaneous storage of multiple ions, either of the same or different species. To determine the influence of ion-ion-interactions [24], we analyzed the data considering only events of one detected ion. Moreover, a count-class analysis [25] was applied and, to be conservative, we added the difference in the ratios in quadrature to the statistical uncertainty. In addition, nonlinear decay in the magnetic field may cause shifts in the system of 0.04(11) ppb/hr [26]; because measurements with $T_{\mathrm{RF}} \approx 2$ s were separated by approximately 1.5 hr, a 0.23 ppb correction was included. Further off-line studies revealed frequency shifts at the level of 1.3 ppb as a result of unbalanced RF excitation stemming from instabilities in the frequency

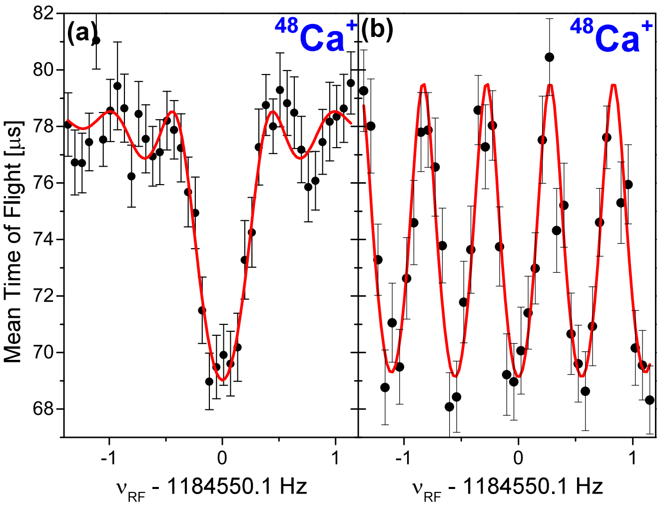

FIG. 1. (Color online) Typical ^{48}Ca resonances using (a) the TOF-ICR technique with $T_{\mathrm{RF}} = 1.953$ s and (b) the Ramsey technique with an excitation scheme of 200-1553-200 ms. The solid line is an analytic fit [9,10] to the data.

TABLE I. $Q_{\beta\beta}$ values of ^{48}Ca and the masses of mother and daughter nuclides were found by interleaving cyclotron-frequency measurements of ^{48}Ca$^+$, ^{48}Ti$^+$, and N^{18}O^{16}O$^+$; the tabulated ratios are the weighted average of seven data sets. The total (statistical and systematic) is listed in parentheses and the statistical uncertainty in square brackets. The last column indicates the precision $\delta R/R$ achieved.

Species	Ratio	Precision
^{48}Ca$^+$-^{48}Ti$^+$	0.999 904 448 9(46)[31]	5×10^{-9}
^{48}Ca$^+$-N^{18}O^{16}O$^+$	1.000 930 621 6(61)[35]	6×10^{-9}
^{48}Ti$^+$-N^{18}O^{16}O$^+$	1.001 026 276 8(47)[41]	5×10^{-9}

generator trigger. As all measured ions were isobars, with identical nominal m/q, they followed the same nominal ion trajectory and experienced the same magnetic and electric fields. Thus, relativistic effects and any mass-dependent effects canceled in the ratio. We varied the excitation times (for conventional excitations $T_{\mathrm{RF}} = 0.457, 1.913, 1.953$ s; for Ramsey 150-653-150 and 200-1553-200 ms) for different data sets to investigate excitation-scheme-dependent effects. In addition, the time window allowed for the dynamic capture of the ion bunch in the Penning trap was varied by -0.5 and $+0.3$ μs from the optimal value to verify the trap compensation (see, e.g., [13]). No statistically significant differences were observed for any of these variations, and all data sets were included in the weighted average. All systematic uncertainties were added in quadrature to the statistical uncertainty and are included in Table I.

III. RESULTS AND DISCUSSION

The ratios R can be related to the $Q_{\beta\beta}$ value and were used to find the masses of Ca and Ti from that of $\mathrm{N}^{18}\mathrm{O}^{16}\mathrm{O}^{+}$ (denoted here as $\mathrm{N}^{18}\mathrm{OO}^{+}$) by

$$Q_{\beta\beta} = (R-1)(M_{\mathrm{Ti}} - m_e) + RB_{\mathrm{Ti}} - B_{\mathrm{Ca}}, \tag{2}$$

$$M_{\mathrm{Ca,Ti}} = R(M_{\mathrm{N^{18}OO}} - m_e) + m_e + RB_{\mathrm{N^{18}OO}} - B_{\mathrm{Ca,Ti}}, \tag{3}$$

where M refers to the atomic mass, m_e the electron mass, B the electronic binding energy of the outermost electron, and the subscripts identify the nuclide. Values for B were taken from [27]. Table II compares the values achieved in this work with values found in recent literature.

The following results could be extracted: We determined for the first time the atomic mass of ^{48}Ti directly using Penning-trap mass spectrometry and found the mass excess to be $-48492.71(21)$ keV; this is a 4.5σ deviation from the Atomic Mass Evaluation (AME) 2012, 0.91(42) keV. We also confirm the mass measurement of ^{48}Ca of [20], which deviates 10.6(4.1) keV from the previous evaluation in 2003 [23]. Finally, we measured the $Q_{\beta\beta}$ value, the most relevant parameter for the $0\nu\beta\beta$ decay, to be 4267.98(32) keV from direct frequency ratios. This value disagrees with the $Q_{\beta\beta}$ value as evaluated in AME 2012, which is based off the Penning-trap mass measurement of ^{48}Ca and indirect mass measurements of ^{48}Ti. Prior to AME 2012, the ISOLTRAP Collaboration measured $M(^{48}\mathrm{Ti})$ with ^{48}TiO molecules and found a value in agreement with the TITAN value. That is, previously the calculated $Q_{\beta\beta}$ value depended on which mass and reaction values were taken, whereas our value is directly and self-consistently determined. More recently, the $Q_{\beta\beta}$ value was measured at the the Low Energy Beam and Ion Trap (LEBIT) facility at the National Superconducting Cyclotron Laboratory (NSCL) [21] to a precision of 79 eV. Our result is in excellent agreement with theirs. With consideration of the LEBIT and ISOLTRAP measurements, we have unambiguously determined that the shift in the $Q_{\beta\beta}$ value is due to an error in the previously accepted atomic mass value of ^{48}Ti.

With an accurate determination of the $Q_{\beta\beta}$ value (and hence phase-space factor), the final ingredient to connect the $0\nu\beta\beta$-decay rate with the neutrino mass is a nuclear matrix element governing the decay. The matrix element is given by

$$M_{0\nu} = M_{0\nu}^{\mathrm{GT}} - \frac{g_V^2}{g_A^2} M_{0\nu}^{F} + M_{0\nu}^{T}, \tag{4}$$

where g_V and g_A are the axial and vector coupling constants, and in addition to the usual Gamow-Teller and Fermi terms, we also include the tensor part, which has been shown to be non-negligible in ^{48}Ca [28]. Of the theoretical methods used to calculate this matrix element, only the nuclear shell model provides an exact treatment of many-body correlations, albeit within a truncated single-particle space (valence space) above an inert core. Though nearly all shell-model Hamiltonians to date rely on phenomenological adjustments to mimic correlations outside the valence space, no modifications are made to the $0\nu\beta\beta$-decay operator. Various predominantly phenomenological many-body calculations for ^{48}Ca currently agree to within a factor of about 3 [29,30]; and, that uncertainty implies the same factor of 3 in an extracted neutrino mass. The effect of correlations outside the valence space on the $0\nu\beta\beta$-decay nuclear matrix element thus remains an open question.

As mentioned earlier, the doubly magic structure and low mass make ^{48}Ca more accessible to *ab initio* many-body methods developed for medium-mass nuclei. Many-body perturbation theory (MBPT) provides a diagrammatic prescription to account for excitations outside the valence space directly from nuclear forces [31,32]. When carried out to sufficiently high order, diagonalization of the resulting *effective* valence-space Hamiltonian, H_{eff}, will reproduce exactly a subset of eigenvalues of the full A-body problem (provided the series converges). Many calculations of ground- and excited-state energies with two-nucleon (NN) and three-nucleon ($3N$) forces in the calcium region exist and agree with each other [33–39], but no attempt has yet been made to calculate the $0\nu\beta\beta$-decay matrix element in ^{48}Ca at the same level of sophistication. MBPT is only now being extended to

TABLE II. A comparison of the $Q_{\beta\beta}$ and mass excesses (ME) determined in this work to recent direct measurements and evaluations. ISOLTRAP had determined the mass of TiO using the reference masses ^{85}Rb and ^{55}Mn as $-48492.9(1.0)$ and $-48492.5(1.2)$ keV respectively; the weighted average is listed below. All values are in keV.

	TITAN	LEBIT	ISOLTRAP	AME 2003	AME 2012
$Q_{\beta\beta}$	4267.98(32)	4268.121(79)		4273.60(4.00)	4266.98(38)
ME(^{48}Ca)	−44224.45(27)	−44224.767(194)		−44214(4)	−44224.759(120)
ME(^{48}Ti)	−48492.70(21)		−48492.3(8)	−48487.7(8)	−48491.734(358)
Ref.	this work	[20,21]	[22]	[23]	[6]

TABLE III. $0\nu\beta\beta$-decay matrix elements $M_{0\nu}$ for ^{48}Ca at various approximations in our many-body framework.

	$M_{0\nu}^{\mathrm{GT}}$	$-\frac{g_V^2}{g_A^2}M_{0\nu}^{F}$	$M_{0\nu}^{T}$	Sum
Bare matrix element $M_{0\nu}$	0.675	0.130	−0.072	0.733
First-order $\hat{X}$ box, no 3p-1h	1.340	0.225	−0.064	1.501
Full first-order $\hat{X}$ box	0.616	0.125	−0.123	0.619
Full second-order $\hat{X}$ box	1.822	0.233	−0.063	1.992
Final matrix element	1.211	0.160	−0.070	1.301

calculate effective two-body operators, as in the case of ^{76}Ge and ^{82}Se [40–42]. We applied this formalism to construct an effective valence-space $0\nu\beta\beta$-decay operator for ^{48}Ca.

We took as our valence space the standard pf shell, consisting of $f_{7/2}$, $p_{3/2}$, $p_{1/2}$, and $f_{5/2}$ orbitals above a ^{40}Ca core. We first constructed the $\hat{X}$ box, an object which includes all "unfolded" diagrams containing the $0\nu\beta\beta$-decay transition operator [42]. At lowest order, $\hat{X}$ is the bare $0\nu\beta\beta$-decay operator, and in the current work, we truncated $\hat{X}$ at second order in the nuclear interaction. To obtain the final effective $0\nu\beta\beta$-decay operator, we included once-folded $\hat{X}$-box diagrams and state norms as in Ref. [42]. The interaction in these diagrams was the *NN* force derived from chiral effective field theory (EFT) at order N^{3}LO [43] and evolved to low momentum (yielding the potential $V_{\mathrm{low}\,k}$) via renormalization group methods [44]. To obtain the nuclear matrix element itself, we combined our effective operator with wave functions calculated from the GXPF1A interaction [45].

Our results for the ^{48}Ca nuclear matrix element appear in Table III, where we list the contributions to the different parts of the operator at various orders in $V_{\mathrm{low}\,k}$. We see the same trends as in ^{82}Se and ^{76}Ge, namely, at first-order, ladder effects increase the total matrix element by a factor of 2, followed by a significant reduction from core-polarization diagrams. Here, however, the effects of second-order diagrams (≈120 in all) and folding are larger, yielding a final value ≈75% larger than that obtained from the bare $0\nu\beta\beta$-decay operator alone. (The increase in ^{76}Ge and ^{82}Se was less than half as much.) We also found that the bare matrix element increased by 8% when we avoided the closure approximation. Although we cannot avoid closure for our effective operator, its matrix element would likely increase by a similar amount.

Though these calculations represent significant progress towards a fully *ab initio* calculation and offer our best estimate for the nuclear matrix element with ^{48}Ca, the large second-order contributions to $\hat{X}$ mean that higher-order contributions could also be significant. Pushing to higher order will be difficult, but we plan other improvements: replacing the phenomenological wave functions by those obtained from an *ab initio* H_{eff}, including the effects of two-body weak currents in the bare operator [46], investigating the size of induced three-body operators [47], and including 3*N* forces in intermediate-state $\hat{X}$-box excitations.

IV. SUMMARY

In conclusion, we provided two improved quantities for ^{48}Ca $0\nu\beta\beta$ decay that together are required to extract the effective Majorana neutrino mass from the decay rate. The $Q_{\beta\beta}$ value is now precisely determined in a self-consistent way and confirms a large deviation from separate determinations. The discrepancy with the accepted ^{48}Ti mass value, uncovered in the recent LEBIT $Q_{\beta\beta}$-value measurement, has been resolved by our mass measurement, revealing a shift of ≈1 keV. The precision achieved herein is below that of the scintillator-based ^{48}Ca $0\nu\beta\beta$-decay experiments and should no longer be a source of systematic error in such data analyses. In addition, we obtained the nuclear matrix element by including the effects of levels outside the valence space in a shell-model calculation. The increases in the $Q_{\beta\beta}$ value and matrix element raise the $0\nu\beta\beta$-decay rate. When they are combined with the improved precision in the $Q_{\beta\beta}$ value, these efforts make a $0\nu\beta\beta$ experiment with ^{48}Ca more attractive.

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