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Atomic mass and double-β-decay Q value of ^{48}Ca

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The possibility of detecting neutrinoless double-β-decay ($0\nu\beta\beta$-decay) in experiments that are currently in operation or under development provides the exciting opportunity to determine the Dirac or Majorana nature of the neutrino and its absolute mass scale. An important datum for interpreting $0\nu\beta\beta$-decay experimental results is the Q value of the decay. Using Penning trap mass spectrometry we have measured the atomic mass of ^{48}Ca to be $M[^{48}\text{Ca}] = 47.952\,522\,76(21)$ u which, combined with the mass of ^{48}Ti evaluated by Audi *et al.* [Nucl. Phys. A **729**, 337 (2003)], provides a new determination of the ^{48}Ca $\beta\beta$-decay Q value: $Q_{\beta\beta} = 4262.96(84)$ keV.

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The confirmation of a nonzero neutrino mass by neutrino oscillation experiments and the range of mixing parameters that they have determined provide for the possibility of detecting neutrinoless double-β-decay ($0\nu\beta\beta$-decay) in experiments that are currently in operation or under development. In addition to a nonzero neutrino mass, this process also requires the neutrino to be a Majorana particle, i.e., its own antiparticle, and that total lepton number is not conserved. The observation of $0\nu\beta\beta$-decay would thus be an indication of physics beyond the Standard Model. Furthermore, a determination of the $0\nu\beta\beta$-decay rate combined with the relevant nuclear matrix elements would give the "effective Majorana mass of the electron neutrino" $\langle m_{\beta\beta}\rangle$, and complementary measurements for a series of different isotopes could give information on the nature of the underlying processes of the interaction, e.g., see Refs. [1,2].

With the exception of a claim by a subset of the Heidelberg-Moscow Collaboration [3], $0\nu\beta\beta$-decay has yet to be observed. The most sensitive experimental limits for the $0\nu\beta\beta$-decay half-life have been set by the Heidelberg-Moscow [4] and IGEX [5] ^{76}Ge experiments, the CUORICINO ^{130}Te experiment [6], and, most recently, the EXO-200 ^{136}Xe experiment [7]. A number of large collaborative efforts are under way to develop and construct next-generation $0\nu\beta\beta$-decay experiments; see Ref. [8] for a recent review. Of these, CANDLES [9] and CARVEL [10] will search for $0\nu\beta\beta$-decay with ^{48}Ca. CANDLES, the successor of the ELEGANT VI experiment [11], which has obtained the most sensitive upper limit for the ^{48}Ca $0\nu\beta\beta$-decay half-life [12], will comprise several tons of CaF_2 detectors and is currently in the prototype stage. CARVEL is a proposal to use isotopically enriched $^{48}\text{CaWO}_4$ crystal scintillators.

The low natural abundance of ^{48}Ca (0.187%) has made it less favorable for $0\nu\beta\beta$-decay experiments than other isotopes. However, ^{48}Ca does have the advantage of having the highest Q value, $Q_{\beta\beta} \approx 4.26$ MeV, of all potential candidates. This results in a large phase-space factor, which enhances the $0\nu\beta\beta$-decay rate and, since it is far higher in energy than γ rays from typical radioactive background sources, ensures a good signal-to-noise ratio.

The $\beta\beta$-decay Q value, defined as the mass difference between the parent and daughter atoms, corresponds to the total energy that is carried away by the two electrons emitted in $0\nu\beta\beta$-decay and hence corresponds to the location of the single peak that would be expected in the sum-energy spectrum of the emitted electrons. It is therefore essential to have a precise and reliable determination of the Q value to a reasonable fraction, i.e., ∼1%, of the detector resolution (the required precision will depend on whether a signal is observed and, if so, the number of counts that are observed). For both CANDLES and CARVEL, the expected energy resolution at 4.27 MeV is 4%. Hence, a Q value determination at the 1 keV level is adequate. In addition, the Q value is required for a precise determination of the phase-space factors $G_{0\nu}$ for $0\nu\beta\beta$-decay and $G_{2\nu}$ for the $2\nu\beta\beta$-decay process allowed by the Standard Model in which two neutrinos and two electrons are emitted. The phase-space factors relate the $\beta\beta$-decay half-life to the nuclear matrix elements via

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

for $2\nu\beta\beta$-decay, and

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

for $0\nu\beta\beta$-decay, where M are the relevant nuclear matrix elements, Z is the nuclear charge, and m_e is the electron rest mass.

In this paper we present a measurement of the mass of ^{48}Ca using Penning trap mass spectrometry which, together with the mass of ^{48}Ti from the most recent published atomic mass evaluation (AME2003) [13], we use to determine the ^{48}Ca $\beta\beta$-decay Q value. Using our new Q value we calculate the phase factors $G_{2\nu}$ and $G_{0\nu}$.

The Low Energy Beam and Ion Trap (LEBIT) facility, located at the National Superconducting Cyclotron Laboratory (NSCL), was the first Penning trap to be used for mass measurements with rare isotopes produced by fast-beam fragmentation [14]. The experimental setup and the methods

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employed have been described in detail elsewhere [15,16] and will be only briefly reviewed here.

The LEBIT Penning trap consists of hyperboloidal ring and end-cap electrodes, and two correction ring and correction tube electrodes that together produce a cylindrically symmetric quadratic electrostatic potential. The electrode structure is immersed in a uniform 9.4 T magnetic field produced by a superconducting solenoid and is aligned along the z axis of the magnet. Inside the Penning trap an ion experiences three normal modes of motion: an axial mode with oscillation frequency f_z and the reduced-cyclotron and magnetron radial modes at frequencies f_+ and f_-, respectively. The two normal-mode radial frequencies are related to the free-space cyclotron frequency for an ion of mass-to-charge ratio m/q in a magnetic field B via $f_c = qB/2\pi m = f_+ + f_-$ [17]. The mass of ^{48}Ca was determined via cyclotron frequency measurements on singly charged ions confined in the Penning trap using a time-of-flight (TOF) resonance technique [18,19], and by calibrating the magnetic field with frequency measurements of the reference ions $^{39,41}\mathrm{K}^+$ or $^{40}\mathrm{Ca}^+$, whose masses are known with high precision.

Calcium and potassium ions were produced by an ion source (Colutron Research Corp.) into which a ceramic charge-holder containing ~50 mg of $^{\mathrm{nat}}$Ca metal was inserted. To operate the source in surface-ionization mode the tungsten filament was positively biased; potassium ions were obtained from impurities in the filament and calcium ions from the vapor from the heated charge. The ratio of potassium to calcium ions produced by the source was optimized by varying the filament current and the location of the calcium charge with respect to the filament. The continuous ion beam produced by the source was directed into a helium-gas-filled radio-frequency quadrupole (RFQ) cooler-buncher [20] for an accumulation period of up to 100 ms, depending on the relative abundance of the isotope being measured. The ions were held in the cooler-buncher for a period of 30 ms then ejected as a microsecond pulse with a well-defined energy and transported to the Penning trap. A fast ion deflector was used as a time-of-flight mass filter, allowing only ions of a given m/q to reach the Penning trap. Any remaining contaminant ions were removed from the Penning trap by applying an rf pulse at their reduced-cyclotron frequency to drive them out of the trap.

The energy of the ion beam after ejection from the cooler-buncher and the capture-timing of ions in the Penning trap were optimized to minimize the ion bunch's axial amplitude in the trap. Finite axial (and radial) ion amplitudes combined with imperfections in the electrostatic trapping potential can result in systematic shifts to the cyclotron frequency. We minimized imperfections in the electrostatic trapping potential using the correction tube and correction ring compensation electrodes by performing a series of measurements in which we looked at shifts to the cyclotron frequency of $^{39}\mathrm{K}^+$ as a function of axial amplitude and for optimized and nonoptimized TOF resonances for different compensation electrode settings, as described in Ref. [21]. To quantify any remaining mass-dependent systematic shift we measured the cyclotron frequency ratios $^{84}\mathrm{Kr}^+/^{84}\mathrm{Kr}^{++}$ and $^{86}\mathrm{Kr}^+/^{86}\mathrm{Kr}^{++}$ before and after taking the $^{48}\mathrm{Ca}^+$ data.

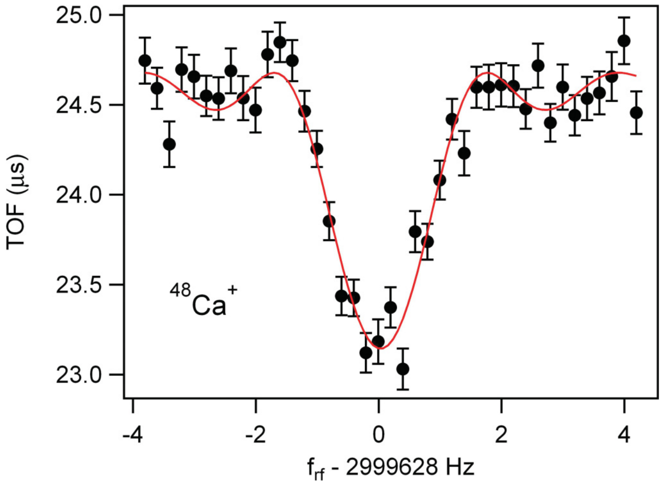

FIG. 1. (Color online) TOF cyclotron frequency resonance for $^{48}\mathrm{Ca}^+$. Each data point is the average TOF to a multichannel plate (MCP) detector for ions ejected from the trap after applying a 500 ms long rf excitation at frequency f_{rf}. The solid curve is a fit of the theoretical line shape to the data.

For each ion, the cyclotron frequency was determined using the conventional TOF resonance technique [18,19] with an excitation time of 500 ms. A typical cyclotron frequency resonance is shown in Fig. 1. Each resonance is the average of 20–40 scans over the frequency range (depending on the count rate of a given isotope from the ion source), took typically 15–30 min, comprised approximately 1000–2000 ions, and provided a single cyclotron frequency measurement with a precision of ~10 ppb (parts per 10^9).

Our data-taking procedure was to encompass each $^{48}\mathrm{Ca}^+$ cyclotron frequency measurement $f_c^{\mathrm{ion}}(t_0)$, where t_0 is the central time of the measurement, with two reference ion measurements, $f_c^{\mathrm{ref}}(t_1)$ and $f_c^{\mathrm{ref}}(t_2)$, at times t_1 and t_2, respectively. The reference ion measurements were first linearly interpolated to determine $f_c^{\mathrm{ref}}(t_0)$ and then the cyclotron frequency ratio (i.e., the inverse mass ratio) $R = f_c^{\mathrm{ion}}(t_0)/f_c^{\mathrm{ref}}(t_0) = m_{\mathrm{ref}}/m_{\mathrm{ion}}$ was obtained. The effects of nonlinear magnetic field drifts over time scales of an individual cyclotron frequency ratio measurement, i.e., ~1 h, have been reduced to <10 ppb by stabilizing the pressure in the liquid helium cryostat of our actively shielded superconducting magnet to 10 parts per 10^6 [16,22], so are negligible. Figure 2(a) shows data for which $^{48}\mathrm{Ca}^+$ and $^{41}\mathrm{K}^+$ were compared over a period of 33 h. The resulting cyclotron frequency ratios and the weighted average are plotted in Fig. 2(b) as the difference $R - R_{\mathrm{ref}}$, where R_{ref} is the inverse mass ratio calculated using $M[^{48}\mathrm{Ca}]$ from Ref. [13] and $M[^{41}\mathrm{K}]$ from Ref. [23].

In between each $^{48}\mathrm{Ca}^+/^{41}\mathrm{K}^+$ measurement we took similar data for $^{48}\mathrm{Ca}^+/^{39}\mathrm{K}^+$ and $^{48}\mathrm{Ca}^+/^{40}\mathrm{Ca}^+$. We took data in this way over the course of a 2 week period with occasional breaks to adjust the ion source to increase the calcium ion output, or to refresh the calcium charge. This procedure naturally broke our data into a series of seven runs similar to the one shown in Fig. 2(a). For each run we obtained the average ratio and statistical uncertainty. The Birge ratios [24] for the individual runs were typically approximately equal to unity. In cases

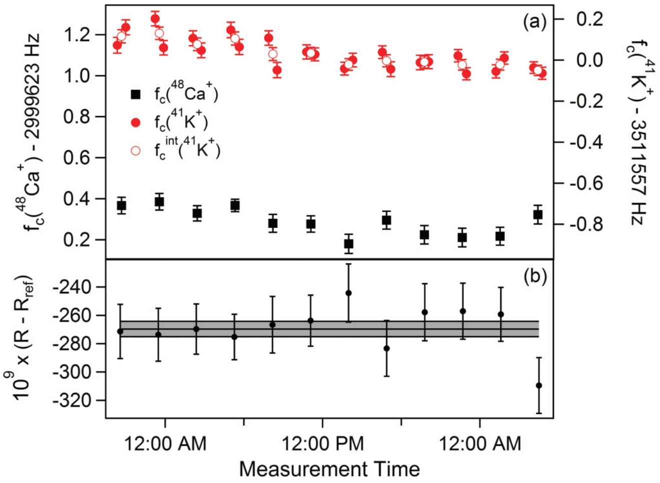

FIG. 2. (Color online) Subset of all cyclotron frequency (inverse mass) ratio data for $^{48}Ca^+/^{41}K^+$. (a) Two $^{41}K^+$ measurements (solid circles) are linearly interpolated (open circles) to obtain the $^{41}K^+$ frequency at the time of the $^{48}Ca^+$ measurement (squares). (b) Each pair of data points is used to obtain a cyclotron frequency ratio measurement, which is compared to the reference ratio (see text). The solid lines show the weighted average and the 1-σ statistical uncertainty band.

where it was greater than unity we increased the statistical error for that run by the Birge ratio. We averaged all seven runs together to obtain the final values for the cyclotron frequency ratios $^{48}Ca^+/^{39}K^+$, $^{48}Ca^+/^{40}Ca^+$, and $^{48}Ca^+/^{41}K^+$ presented in Table I.

The systematic uncertainties assigned to the ratios were determined from three separate sources. First, from our $^{84}Kr^+/^{84}Kr^{++}$ and $^{86}Kr^+/^{86}Kr^{++}$ cyclotron frequency comparisons: these ratios involved measurements between ions with m/q differences of 42 and 43 u/e, which are ~5–6 times larger than for $^{48}Ca^+/^{39,41}K^+$ or $^{40}Ca^+$. Our ratios for the ^{84}Kr and ^{86}Kr measurements differed from the calculated m/q ratios by $5.0(5.5) \times 10^{-9}$ and $8.6(6.7) \times 10^{-9}$, respectively. Since these results showed no statistically significant shift we did not use them to apply corrections to the ratios given in Table I, but instead used them to estimate an uncertainty of 0.19×10^{-9}/u due to comparing ions of different m/q and determined the corresponding systematic uncertainties for the three frequency ratios. We also note that from the ^{84}Kr and ^{86}Kr data we were able to extract the cyclotron frequency ratios $^{84}Kr^+/^{86}Kr^+$ and $^{84}Kr^{++}/^{86}Kr^{++}$. Both results agreed with the mass ratios obtained using the high-precision mass values for ^{84,86}Kr measured with the Florida State University (FSU) Penning trap [25].

TABLE I. Average cyclotron frequency (inverse mass) ratios (with combined statistical and systematic uncertainties in parentheses) for $^{48}Ca^+$ compared against three reference ions. σ_{stat} and σ_{syst} are the statistical and systematic uncertainties, respectively.

Ion pair	$\sigma_{stat} \times 10^{-9}$	$\sigma_{syst} \times 10^{-9}$	Ratio
$^{48}Ca^+/^{39}K^+$	2.6	2.9	0.812 545 439 0(39)
$^{48}Ca^+/^{40}Ca^+$	2.9	2.8	0.833 376 371 4(40)
$^{48}Ca^+/^{41}K^+$	2.7	2.8	0.854 214 605 5(39)

Second, we took data while we systematically varied either the radial or axial amplitude of the ions and looked for shifts to the cyclotron frequency. We saw no shift to f_c as a function of radial amplitude over a range between half and two times the amplitude used in our $^{48}Ca^+$ data. From our f_c vs axial amplitude data and based on the 25 ns resolution of our ion-capture timing sequence (which we optimized with a separate procedure to minimize the axial amplitude of the ion), we estimated systematic uncertainties of 1.25, 1.30, and 1.35 × 10^{-9} to apply to the ratios $^{48}Ca^+/^{39}K^+$, $^{48}Ca^+/^{40}Ca^+$, and $^{48}Ca^+/^{41}K^+$, respectively.

Finally, there is also the possibility of systematic frequency shifts due to the Coulomb interaction when there is more than one ion of a given species in the trap (unwanted ions of other species were removed by an rf dipole excitation at their modified-cyclotron frequency, f_+, to drive them out of the trap). To investigate this effect we cut the data to exclude measurements for which a given limit on the number of ions recorded on the MCP detector was exceeded, and determined the average cyclotron frequency ratio as before. We performed this analysis with limits of between two and ten detected ions and, averaging the results for the three ratios we measured, we determined the shift due to this effect to be $0.21(27) \times 10^{-9}$/detected ion. For the maximum of six detected ions per shot used in the final data set, this result was used to estimate an additional systematic uncertainty of 2.0×10^{-9} to include for each ratio. All three contributions to the systematic uncertainty were added in quadrature and are listed in Table I.

Using the average cyclotron frequency ratios given in Table I, accounting for the mass of the missing electrons (the effect of electron binding energies is negligible at this level of precision), and using values for the masses of ^{39}K and ^{41}K measured with the FSU trap [23], and the mass of ^{40}Ca measured at SMILETRAP [26,27], we obtained three values for the mass of ^{48}Ca. These results, along with their weighted average are given in Table II. Our final result is $M[^{48}\mathrm{Ca}] =$ 47.952 522 76(21) u, which corresponds to a mass excess of −44224.767(194) eV. This result differs from the AME2003 value [13] by −10.64(4.08) keV but agrees with the value determined in a recent unpublished preliminary update to the

TABLE II. Atomic mass of ^{48}Ca, in u, and corresponding mass excess, in keV, obtained from the cyclotron frequency ratios given in Table I, their weighted average, and results from the most recent publication of, and an unpublished update to, the atomic mass evaluation.

Source	Mass (u)	Mass excess (keV)
$^{48}Ca^+/^{39}K^+$	47.952 522 75(23)	−44 224.771(214)
$^{48}Ca^+/^{40}Ca^+$	47.952 522 80(23)	−44 224.725(218)
$^{48}Ca^+/^{41}K^+$	47.952 522 72(22)	−44 224.798(202)
Avg.	47.952 522 76(21)	−44 224.767(194)
AME2003 [13]	47.952 534 18(438)	−44 214.13(4.08)
AME2011 [28]	47.952 524 13(234)	−44 223.49(2.18)

AME (AME2011) [28] and improves on the uncertainty of these two values by factors of 21 and 11, respectively.

Combining our result for $M[^{48}\mathrm{Ca}]$ with the value for $M[^{48}\mathrm{Ti}] = 47.947\ 946\ 28(88)$ u from the AME2003 [13], we determine the ^{48}Ca $\beta\beta$-decay Q value to be 4262.96(84) keV, where the uncertainty is dominated by the uncertainty in the mass of ^{48}Ti. Our new value for the ^{48}Ca $\beta\beta$-decay Q value is 10.64(4.00) keV lower in energy than the AME2003 value. We note that the preliminary AME2011 [28] indicates an adjustment to the mass of ^{48}Ti to 47.947 941 95(38) u, corresponding to a mass excess of $-48491.77(35)$ keV. Using this value for $M(^{48}\mathrm{Ti})$ we obtain a ^{48}Ca $\beta\beta$-decay Q value of 4267.00(40) keV. This result differs from our Q value obtained using the AME2003 ^{48}Ti mass by 4.04(93) keV, partially compensating for the 10.64 keV reduction in the Q value due to our new ^{48}Ca mass measurement. Using the two Q values given above and following the procedure described in Ref. [29] using $g_A = 1.254$, we calculate two values for each of the phase-space factors $G_{2\nu}$ and $G_{0\nu}$, corresponding to the $2\nu\beta\beta$-decay and $0\nu\beta\beta$-decay modes, respectively. The results, given in Table III, show a 0.9% and a 0.4% difference between the two Q values for $G_{2\nu}$ and $G_{0\nu}$, respectively. We note that reevaluated phase-space factor calculations that make use of exact Dirac wave functions with finite nuclear size and electron screening have recently been performed by Kotila and Iachello [30]. However, for light nuclei such as ^{48}Ca these new results do not differ significantly from those obtained by earlier methods [30].

TABLE III. Q values determined using the mass of ^{48}Ca from this work and the mass of ^{48}Ti from Refs. [13,28], and corresponding phase-space factors for $2\nu\beta\beta$-decay and $0\nu\beta\beta$-decay calculated following Ref. [29].

^{48}Ti [Ref.]	Q value (keV)	$G_{2\nu}$ ($\times 10^{-17}$ yr^{-1})	$G_{0\nu}$ ($\times 10^{-14}$ yr^{-1})
AME2003 [13]	4262.96(84)	3.892(7)	6.477(5)
AME2011 [28]	4267.00(40)	3.927(4)	6.502(3)

Using Penning trap mass spectrometry we have measured the atomic mass of ^{48}Ca to a precision of <200 eV and found a 10.6 keV shift with respect to the previously accepted value. By combining our result with that for the mass of ^{48}Ti, we have provided a new determination of the ^{48}Ca $\beta\beta$-decay Q value. However, a preliminary update to the global evaluation of atomic masses indicates that the previously accepted value for $M[^{48}\mathrm{Ti}]$ should also be adjusted by 4.1 keV. Recent Penning trap measurements [31] with ISOLTRAP of the mass ratios $M(^{48}\mathrm{Ti}^{16}\mathrm{O}^{+})/M(^{85}\mathrm{Rb}^{+})$ and $M(^{48}\mathrm{Ti}^{16}\mathrm{O}^{+})/M(^{55}\mathrm{Mn}^{+})$ contributed to the adjusted ^{48}Ti mass in the AME2011. The two ratios each provide a $M[^{48}\mathrm{Ti}]$ determination to a precision of $\sim$1 keV and agree with each other, but their average differs from the AME2011 mass value by more than one standard deviation. Hence, a further Penning trap measurement of the mass of ^{48}Ti to sub-keV precision would still be desirable.

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