Double-magicity of $^{52}\text{Ca}$ resolved by precision mass measurements of neutron-rich scandium isotopes around $N = 32$

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We report high-resolution mass measurements of $^{50-55}\text{Sc}$ isotopes performed at the LEBIT facility at NSCL and at the TITAN facility at TRIUMF. Our results provide a substantial reduction of their uncertainties and indicate significant deviations, up to 0.7 MeV, from the previously recommended mass values for $^{53-55}\text{Sc}$. Our analysis reveals that the trends of the closed shell effects in the semimagic $N = 32$ isotope conform to typical shell evolution, and confirms that empirical shell gaps peak at the doubly-magic $^{52}\text{Ca}$, and not at $^{54}\text{Sc}$ as a previous analysis suggests. The results of this work represent the last missing piece for a detailed description of shell effects on the binding energies at $N = 32$ above $Z = 20$. Further, we discuss potential implications for the theoretical description of the neighboring emerging shell, at $N = 34$.

The formation of simple, periodic patterns is key to understanding the organization of countless many-body systems \[1\]. In the case of the atomic nucleus, the formation of shell-like structures at certain “magic” nucleon numbers (like 2, 8, 20, 28, 50...) \[2\] constitutes the foundation of our understanding of the structure of these objects. Once believed to be immutable, these shells are now known to appear or vanish in extreme cases of proton-to-neutron ratio \[3\]. The appearance and evolution of emerging shell effects have become standard metrics to benchmark nuclear theories.

While the appearance of closed shell behaviors at neutron number $N = 32$ in the vicinity of proton number $Z = 20$ is very well established, its study continues to be of significant scientific interest. It has been studied through several observables, such as nuclear masses \[4-9\], excitation energies \[10-14\] and transition probabilities \[15-19\]. Theoretically, it has been well described by both phenomenological shell model approaches \[17\] and \textit{ab initio} many-body quantum methods \[18\]. Thus, $^{52}\text{Ca}$ is expected to have enhanced shell effects for being both proton magic ($Z = 20$) and neutron magic ($N = 32$). This can be observed, for example, in the systematics of $2^+$ excitation energies in even-even nuclei, where $^{52}\text{Ca}$ exhibits the highest value among all documented $N = 32$ isotones \[13,19\].

In contrast, a few recent results challenge the doubly-magic nature of $^{52}\text{Ca}$. First, a laser spectroscopy measurement of $^{52}\text{Ca}$ revealed its unexpectedly large charge radius \[20\], which conflicts with the notion that magic nuclei are especially compact \[21\]. Moreover, Isochronous Mass Spectrometry (IMS) measurements of neutron-rich scandium isotopes ($Z = 21$) suggest the empirical neutron shell gap at $N = 32$ is unexpectedly higher in Sc than in the proton-magic chain \[7,22\].

In this letter, we revisit the enlarged shell gap among scandium isotopes, which is the only isotopic chain above $Z = 20$ still unexplored using high-resolution techniques. We report precision mass measurements of $^{50-55}\text{Sc}$, performed in a joint collaboration between experimental groups at the National Superconducting Cyclotron Laboratory (NSCL) in the U.S. and at the TRIUMF National Laboratory in Canada. With our results, the mass surface around $N = 32$ reveals a smooth evolution of the shell gaps at the $N = 32$ isotope, and confirms that empirical shell gaps indeed peak at the doubly-magic $^{52}\text{Ca}$.

The neutron-rich isotopes $^{50-53}\text{Sc}$ were produced at NSCL and measured at the Low Energy Beam and Ion Trap (LEBIT) facility \[23\]. The samples were produced in flight by nuclear fragmentation of a $^{76}\text{Ge}$ primary ion beam, that was accelerated to 130 MeV/u by NSCL’s Coupled Cyclotron Facility and impinged on a natural Be target of about 0.4 g/cm$^2$ thickness. The beam was purified at the A1900 fragment separator \[24\] and delivered to the NSCL’s gas catcher \[25\], where the high-energy fragments were stopped in a high-purity He gas. The ions...
were extracted at low energies from the gas cell and selected in mass-to-charge ratio \((A/Q)\) by a dipole magnet. The species of interest were extracted as singly charged molecules, mostly oxides, formed during stopping in the gas cell. The ion beam was then delivered to the LEBIT facility \cite{23}, where the experiment was performed.

LEBIT is an ion trap facility dedicated to perform high-precision mass spectrometry of short-lived ions \cite{23}. The beam was received into LEBIT’s cooler and buncher \cite{26}, where the continuous rare isotope beam was converted into short low-emittance pulses, optimized for further injection into ion traps. The ion pulses were then sent to LEBIT’s 9.4 T Penning trap mass spectrometer \cite{27}, where they were confined following a motion that is well described in the literature \cite{28, 29}. The ion bunch was further purified against isobaric contaminants by applying a dipolar radio-frequency field \cite{29, 30}.

The measurement of the mass \((m)\) of the ion is done through the measurement of the frequency \((\nu)\) of the cyclotron motion about the trap’s magnetic field: \(\nu = (q B)/(2\pi m)\), where \(q\) is the charge of the ion and \(B\) is the strength of the magnetic field. To measure \(\nu_e\), we employed the Time-of-Flight Ion-Cyclotron-Resonance technique (ToF-ICR), using standard excitation schemes ranging between 50 ms and 500 ms. Figure 1a shows a typical ToF-ICR spectrum obtained in the procedure. Details on this technique can be found in \cite{29}.

The calibration of \(B\) was done through the measurement of the cyclotron frequency of a reference ion \((\nu_{c,\text{ref}})\), whose mass is well documented in the literature \cite{31}. The reference ions were all well-known molecular ions produced in the gas catcher and delivered with the ion of interest, with the same \(A/Q\), to avoid mass-dependant systematic deviations. Measurements of \(\nu_{c,\text{ref}}\) were performed at intervals not longer than 1.5 hour, interleaved between measurements of \(\nu_c\) of ions of interest, to account for time variations in the magnetic field.

The analysis of ToF-ICR spectra followed similar procedures as other experiments performed at LEBIT, for example as in \cite{32}, and is only briefly described here. Each spectrum was fitted with an analytical function described in \cite{29}, from which the cyclotron frequency was obtained. A count-class analysis \cite{33} was performed to account for frequency shifts due to ion-ion interaction.

The atomic mass of the species of interest \((m_e)\) was determined through the cyclotron frequency ratio \((R)\) between the ion of interest and the reference ion: \(R = \nu_{c,\text{ref}}/\nu_c = (m_a - m_e)/(m_{\text{ref}} - m_e)\), where \(m_e\) is the mass of the electron and \(m_{\text{ref}}\) is the mass of the reference species (obtained from \cite{31}, summing the masses of all atoms of the molecule). This equation is valid for singly ionized species and it disregards insignificant electron and molecular binding energies. \(\nu_{c,\text{ref}}\) was obtained from an interpolation between the reference measurements before and after the ToF-ICR measurement of the ion of interest. The mass of the nuclide of interest is obtained by subtracting the masses of its molecular counterparts.

The masses of \(^{54}\text{Sc}\) and \(^{55}\text{Sc}\) were measured at TRIUMF’s Ion Trap for Atomic and Nuclear science (TITAN) facility \cite{34}. These measurements were part of an experimental campaign that aimed to extend past successful results in the same region \cite{8, 9}, and therefore follow very similar procedures. Further results of this campaign will be reported in a future publication.

The samples were produced via the ISOL method through spallation reactions at TRIUMF’s Isotope Separator and ACcelerator (ISAC) \cite{35} facility by impinging a 480 MeV proton beam of 50 µA onto a Ta target, 22.7 g/cm² thick. The reaction products were stopped and thermalized in the target material, released through desorption, and surface ionized at the TRILIS ion source \cite{36}. The beam was extracted from the target, selected in \(A/Q\) at ISAC’s dipole mass separator \cite{37} and delivered at low energy to the TITAN facility \cite{34}.

TITAN, similarly to LEBIT, is an ion-trap facility dedicated to perform mass spectrometry of short-lived ions \cite{34}. It employs two mass spectrometers, a Penning Trap Mass Spectrometer \cite{38} and a Multiple-Reflection Time-of-Flight Mass Spectrometer (MR-TOF-MS) \cite{39}. In this experiment, the radioactive beam from ISAC was accumulated at TITAN’s cooler and buncher \cite{40} for 20 ms and sent as ion bunches to the MR-TOF-MS.
TABLE I. Results of the mass measurements performed. The mass excesses are relative to the atomic mass of the nuclides of interest. The mass relationship between ion of interest and reference ion depends on the technique, for the LEBIT ToF-ICR data it is the average frequency ratio (R), for the TITAN MR-TOF-MS data it is the mass difference. The results are also compared to the mass excesses recommended by the AME16 [31]. All masses are in keV/c².

| Facility | Nuclide | Ion of Interest | Reference Ion | Mass Relationship | Mass Excess | Literature | Difference |
|----------|---------|-----------------|---------------|-------------------|-------------|------------|------------|
| LEBIT    | $^{50}$Sc | $^{54}$Sc $^{16}$O $^+$ | $^{12}$C$^{35}$F$^{98}$Cl $^+$ | 0.999 694 485 (41) | $-44537.1 (2.5)$ | -44547 (15) | 10 (15) |
|          | $^{51}$Sc | $^{56}$Sc $^{16}$O $^+$ $^{34}$S$^{35}$F$^{16}$O $^+$ | 0.999 875 402 (39) | $-43250.4 (2.5)$ | -43229 (20) | -22 (20) |
|          | $^{52}$Sc | $^{57}$Sc $^{16}$O $^+$ $^{34}$S$^{35}$F$^{16}$O $^+$ | 0.999 803 339 (48) | $-40523.6 (3.0)$ | -40443 (82) | -80 (82) |
|          | $^{53}$Sc | $^{58}$Sc $^{16}$O $^+$ $^{34}$S$^{35}$F$^{16}$O $^+$ | 0.999 885 577 (270) | $-38769 (17)$ | -38907 (94) | 138 (96) |
| TITAN    | $^{54}$Sc | $^{54}$Sc $^{16}$O $^+$ | $^{16}$O $^+$ | 22497 (14) | $-34438 (14)$ | -33891 (270) | -547 (270) |
|          | $^{55}$Sc | $^{55}$Sc $^{16}$O $^+$ | $^{16}$O $^+$ | 24268 (62) | $-30842 (62)$ | -30159 (450) | -683 (460) |

The MR-TOF-MS determines the mass of a charged particle through time-of-flight [41,42]. This device extends the flight path by confining the ion between a pair of electrostatic mirrors while preserving the initial time spread. In this experiment, the bunches were received by the MR-TOF-MS in an internal ion preparation system, where ions were re-cooled for about 13 ms. The ions were then sent to the mass analyser for time of flight of about 7.5 ms, where they underwent 520 isochronous turns between the mirrors. Finally, they were detected by a MagnetoTOF detector [43]. A mass-range selector, similar to [45], was used to account for drifts in time of flight, and the average count rate was kept below 2 counts/cycle.

In both spectra taken with $A/Q = 54$ and 55, we identified the presence of isobaric singly charged Cr, Fe, Mn, V, Ti, and Sc, as well as of certain molecules. A typical time of flight spectrum is shown in figure 1b. Every peak in the MR-TOF-MS spectra was fitted using a Gaussian function. The spectra were mass calibrated using the nonrelativistic relationship: $m/q = c (t_{tof} - t_0)^2$, where $c$ and $t_0$ are calibration constants and $t_{tof}$ is the fitted centroid of the peak. The parameter $t_0$ is a constant delay caused in the signal processing and was determined through offline measurements. Stable $^{54,55}$Cr$^+$ formed dominant peaks in their spectra and, therefore, were chosen as suitable calibrants for $c$ using their atomic mass values available in the literature [31]. A time-dependent calibration, similar to [45], was used to account for drifts in time of flight.

The atomic masses of the species of interest were determined through the relationship $m_n = m + m_e$, which disregards electron binding energies. A relative systematic uncertainty of $3 \times 10^{-7}$ was added following the prescription outlined in previous experiments [8,9,50], as well as an additional relative uncertainty of $1.9 \times 10^{-7}$ to account for ion-ion interaction effects [47].

The masses obtained in both experiments are reported in table 1. The precision was improved in all cases, some by over an order of magnitude, to the scale of a few tens of keV. Our measurements are compatible, within 2.0 $\sigma$, with previous experimental results employing moderate-resolution techniques, including the two most recent [7,48]. These two are re-analysis of data acquired in previous experiments [22,49], which dominate the recommended values by the Atomic Mass Evaluation of 2016 (AME16) [31]. Despite the 2.0 $\sigma$ compatibility with previous experiments, our updated values represent deviations up to 0.7 MeV from the AME16 values and values combining our results and results from other recent experiments [7,9,31,48,50].

Consecutive sharp features are seen at $N = 28$, a “canonical” magic number, and at $N = 32$, an “emerging” magic number. Our results confirm the strong shell effects in $^{53}$Sc, but provide a lower shell gap (3.45 ± 0.06 MeV), $2\sigma$ from the AME16 and the most recent experimental result [7] (4.4 ± 0.5 MeV).

Our update to the empirical shell gap of $^{53}$Sc considerably impacts the evolution of the $N = 32$ shell closure. Figure 2c shows $\Delta_{2n}(Z,N)$ for scandium isotopes using AME16 values and values combining our results and results from other recent experiments [7,9,31,48,50]. Consecutive sharp features are seen at $N = 28$, a “canonical” magic number, and at $N = 32$, an “emerging” magic number. Our results confirm the strong shell effects in $^{53}$Sc, but provide a lower shell gap (3.45 ± 0.06 MeV), $2\sigma$ from the AME16 and the most recent experimental result [7] (4.4 ± 0.5 MeV).

We analyzed the robustness of these trends by comparing the shell gap data with state-of-the-art models. We chose four theoretical approaches that had great success in describing shell effects at $N = 32$. Among ab initio approaches, we employed Valence-Space In-Medium Similarity Renormalization Group [51,52] (VS-IMSRG) cal-
Theoretical predictions are highly disparate regarding the description of the \( N = 34 \) shell gap. Although mass data are not refined enough to provide a clear description, shell gaps at \( N = 34 \) do not indicate any meaningful shell effect at \( Z \geq 20 \). However, experimental values seem to lie in between predictions using the KB3G and the GX1A Hamiltonians, which can also be seen less pronouncedly at \( N = 32 \) around its peak. A similar discrepancy has also been observed in descriptions of \( 2^+ \) excitation energy using these interactions [19, 62, 63]. The \( 2^+ \) state of \( ^{54}\text{Ca} \) lies 2.04(2) MeV above the ground state. According to our calculations with the GX1A interaction, it lies at 2.96 MeV, while KB3G predicts 1.34 MeV. The VS-IMSRG calculations are in better agreement with data in the \( Z \leq 22 \) region, but predict the shell gap to reduce towards argon (\( Z = 18 \)). It suggests a conflict with recent \( \gamma \)-spectrometry results, that indicate the start of \( N = 34 \) shell effects is at Ca (\( Z = 20 \)) [19] but overcoming \( N = 32 \) in strength at Ar (\( Z = 18 \)) [13, 58].

In summary, we performed high-precision mass measurements of \(^{50–54}\text{Sc}\) at the LEBIT facility at NSCL and of \(^{54,56}\text{Sc}\) at the TITAN facility at TRIUMF. With our mass values, we obtained a smooth and monotonic evolution of the \( N = 32 \) shell gaps above \( Z = 20 \), finally completing the mass description of the emergence of this closed shell using high-resolution methods. The observed behavior conforms to typical shell evolution as confirmed by various theoretical predictions, both from phenomenological and \textit{ab initio} approaches. Our results

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{\text{AME16/ This work}}
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FIG. 3. Measured (coloured lines, same as figure 2) and predicted (black lines) shell gaps for several isotones in the region of interest: the magic $N = 28$, the non-magic $N = 30$, the semi-magic $N = 32$, and the possibly magic $N = 34$.

support $^{52}\text{Ca}$ as a doubly-magic nucleus, establishing it as the peak of empirical shell gaps instead of $^{53}\text{Sc}$, as a previous analysis suggested. Our analysis also explored some theoretical approaches that have had superior performance in describing shell effects in the $N = 32$ isotope. The existing discrepancies among them can be associated with larger deviations in the description of emerging shell effects at $N = 34$. Therefore, given the intimate relationship between the closed shell behaviors at $N = 32$ and $N = 34$, we encourage continuous exploration of this region using high-resolution mass spectrometry techniques, both towards the higher-$N$ and lower-$Z$ boundaries.

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