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## Improved Upper Limit on the Neutrino Mass from a Direct Kinematic Method by KATRIN

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We report on the neutrino mass measurement result from the first four-week science run of the Karlsruhe Tritium Neutrino experiment KATRIN in spring 2019. Beta-decay electrons from a high-purity gaseous molecular tritium source are energy analyzed by a high-resolution MAC-E filter. A fit of the integrated electron spectrum over a narrow interval around the kinematic end point at 18.57 keV gives an effective neutrino mass square value of  $(-1.0^{+0.9}_{-1.1})$  eV<sup>2</sup>. From this, we derive an upper limit of 1.1 eV (90% confidence level) on the absolute mass scale of neutrinos. This value coincides with the KATRIN sensitivity. It improves upon previous mass limits from kinematic measurements by almost a factor of 2 and provides model-independent input to cosmological studies of structure formation.

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Introduction.—The observation of flavor oscillations of atmospheric and solar neutrinos [1,2] as well as oscillation studies at reactors and accelerators unequivocally prove neutrinos to possess nonzero rest masses (e.g., [3]), contradicting the standard model (SM) expectation of them being massless. The absolute values  $m_i$  of the neutrino mass states  $\nu_i$  (*i* = 1, 2, 3), which cannot be probed by oscillations, are of fundamental importance in cosmological studies [4–6] and for particle physics models beyond the SM [7].

Because of the unique role of primordial neutrinos in the formation of large-scale structures in the universe, observations of matter clustering in different epochs of the universe allow one to probe the neutrino mass sum  $\Sigma_i m_i$ . The current upper limits depend on the selection of data sets included in the analyses and are valid only within the ACDM concordance model [6,8]. Another modeldependent method is provided by the search for neutrinoless double beta decay  $0\nu\beta\beta$ , a process forbidden in the SM due to lepton number violation. It gives access to the effective Majorana neutrino mass (e.g., [9,10]).

A model-independent, direct method for probing the neutrino mass scale in the laboratory is provided by kinematic studies of weak-interaction processes such as  $\beta$  decay of tritium (<sup>3</sup>H) and electron capture on holmium (<sup>163</sup>Ho) [11–15]. These investigations yield an incoherent sum of spectra, containing the squares of the neutrino eigenmasses  $m_i^2$  as parameters. Each spectral component is weighted by the absolute square of the corresponding electron-flavor matrix element  $|U_{ei}|^2$ . In the quasidegenerate regime  $m_i > 0.2$  eV, the eigenmasses are the same to better than 3%. The mass measured in  $\beta$  decay or electron capture, often called " $m(\nu_e)$ ," is the neutrino mass  $m_\nu \approx m_i$ in this regime.

Because of its low end point energy ( $E_0 = 18.57 \text{ keV}$ ) and favorable half-life ( $t_{1/2} = 12.32$  yr), the decay of tritium  ${}^{3}\text{H} \rightarrow {}^{3}\text{He}^{+} + e^{-} + \bar{\nu}_{e}$  has been investigated by a large number of experiments looking for the small, characteristic shape distortion of the  $\beta$  spectrum close to  $E_0$  due to  $m_{\mu}$ [11,12]. Experimental advances over many decades have steadily increased the sensitivity to the present upper limit of  $m_{\nu} < 2 \text{ eV}$  (95% confidence level, C.L.) [16]. In this Letter, we report on the first neutrino mass result from the Karlsruhe Tritium Neutrino experiment KATRIN [17-20], which is targeted to advance the sensitivity on  $m_{\nu}$  by 1 order of magnitude down to 0.2 eV (90% C.L.) after five years.

Experimental setup.—KATRIN combines a windowless gaseous molecular tritium source (WGTS), pioneered by

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FIG. 1. The major components of the KATRIN beam line consist of (a) the rear section for diagnostics, (b) the windowless gaseous tritium source WGTS, c) the pumping section with the DPS and CPS cryostats, and a tandem setup of two MAC-E-filters: (d) the smaller prespectrometer and (e) the larger main spectrometer with its surrounding air coil system. This system transmits only the highest-energy  $\beta$  decay electrons onto (f) the solid-state detector where they are counted.

the Los Alamos experiment [21], with a spectrometer based on the principle of magnetic adiabatic collimation with electrostatic filtering (MAC-E-filter) [22,23], developed at Mainz and Troitsk [24,25]. These techniques allow the investigation of the end point region of tritium  $\beta$  decay with very high energy resolution, large statistics, and small systematics. KATRIN has been designed and built to refine this direct kinematic method to its ultimate precision level. To improve the sensitivity on  $m_{\nu}$  by 1 order of magnitude calls for an increase in statistics and a reduction of systematic uncertainties by 2 orders of magnitude, as the observable in kinematic studies is the neutrino mass square,  $m_{\nu}^2$ .

Figure 1 gives an overview of the 70 m long experimental setup located at the Karlsruhe Institute of Technology. The source-related components in contact with tritium, the rear section (RS) (a), the WGTS cryostat (b), as well as the differential (DPS) and cryogenic (CPS) pumping sections (c) are integrated into the extensive infrastructure of Tritium Laboratory Karlsruhe to enable a closed cycle of tritium [26]. High-purity tritium gas from a pressure-controlled buffer vessel is continuously injected at 30 K into the WGTS at the midpoint of its 90 mm diameter, 10 m long stainless steel beam tube. The gas then diffuses to both ends where it is pumped out by a series of turbomolecular pumps (TMPs) in the DPS, yielding the nominal column density  $\rho d_{\rm nom} = 5 \times 10^{17}$  molecules cm<sup>-2</sup>. In combination with the CPS, housing a large-capacity cryotrap operated at around 3 K, the flow rate of tritium into the following spectrometer and detector section [Figs. 1(d)-1(f)] downstream is negligible, well below the 14 orders of magnitude of flow reduction required to eliminate source-related background by neutral tritium gas [17].

The source magnetic field (section b) in Fig. 1,  $B_{\text{WGTS}} = 2.52 \text{ T}$ ) as well as other superconducting solenoids [section (c) in Fig. 1] [27] adiabatically guide primary  $\beta$ -decay electrons, secondary electrons, and ions to the spectrometers. A series of blocking and dipole electrodes eliminates ions by an  $\vec{E} \times \vec{B}$  drift to the beam tube, so that they cannot generate background in the spectrometer section [19]. High-precision electron spectroscopy is achieved by the MAC-E-filter technique, where electrons of charge q are guided by the magnetic field, collimated by its gradient and filtered by an electrostatic barrier, the retarding potential energy qU. The resulting high-pass filter transmits only electrons with enough energy to overcome the barrier qU and allows the scanning of the tritium  $\beta$ -decay spectrum in an integral mode.

The tandem configuration of MAC-E-filters performs a two-step filter process: first, the smaller prespectrometer is operated at fixed high voltage (HV) of -10.4 kV in this work to act as a prefilter to reject electrons that carry no information on  $m_{\nu}$ . In a second step, a variable qU is applied to the main spectrometer for precision filtering of  $\beta$ -decay electrons close to  $E_0$ . Its huge size guarantees fully adiabatic motion to the central "analyzing plane," where the minimum magnetic field  $B_{\min}$  and the maximum retarding energy qU coincide for the filtering process to occur. Elevating the two spectrometers to a negative HV forms a strong Penning trap which can give rise to background [28,29]. This is avoided by operating both at an ultrahigh vacuum (UHV) regime of  $10^{-11}$  mbar using nonevaporable getter (NEG) pumps and TMPs [30].

A defining property of a MAC-E-filter is  $\Delta E/E$ , the filter width at energy *E*, which is given by the ratio  $B_{\min}/B_{\max}$  of the minimum to maximum magnetic field in nonrelativistic approximation. The present ratio (0.63 mT/4.24 T) is equivalent to  $\Delta E = 2.8$  eV at  $E_0$ . This value constrains the size  $V_{\text{ft}}$  of the flux tube around  $B_{\min}$  and, consequently, the overall background rate, which is proportional to  $V_{\text{ft}}$ to the first order. A large air coil system of 12.6 m diameter [31] is used to adjust  $B_{\min}$  and  $V_{\text{ft}}$ . After the potential of the spectrometer vessel is elevated, an offset of up to -200 V can be applied to the wire electrode system mounted on the inner surface of the vessel to define qU.

Electrons transmitted through the spectrometers are finally counted in a radially and azimuthally segmented monolithic silicon detector array with 148 pixels [32] as a function of qU. To optimize the signal-to-background ratio, transmitted electrons are postaccelerated by a potential of +10 kV before they impinge on the detector.

*Commissioning measurements.*—Over the past years, we have commissioned the entire setup by a series of dedicated long-term measurements [19,26,27,33] which have demonstrated that all specifications [18] are met, or even surpassed by up to 1 order of magnitude, except for the background rate  $R_{bg}$ .

A major benchmark is to operate the source at  $\rho d_{nom}$  at a stability level of  $10^{-3}$ /h so that variations of the column density  $\rho d$  can be neglected. This calls for a stable gas injection rate via capillaries [26] and a constant beam-tube temperature. For the latter, a stability level of better than  $10^{-3}$ /h has been achieved by a two-phase beam-tube cooling system at 30 (100) K using neon (argon) as a cooling fluid [34]. In mid-2018, measurements at 1% DT concentration within a 99% D<sub>2</sub> carrier gas at  $\rho d_{nom}$  have verified the required level of source stability [35]. This "first tritium" campaign has allowed us to collect the first integral electron spectra which agree well with the model expectation.

In this spectral comparison, the response function f(E - qU) [20] plays a fundamental role [see Eq. (1)], as it converts the theoretical  $\beta$  spectrum into the experimental spectrum. It describes the probability of transmission of an electron with initial energy *E* as a function of its surplus energy E - qU. For an ensemble, it depends on the angular spread of electrons and the amount of neutral gas they pass in the source, where they can undergo inelastic scattering processes with a total cross section  $\sigma$  (3.64 × 10<sup>-18</sup> cm<sup>2</sup> at 18.57 keV, adopted from [36]).

We measure f(E - qU) using monoenergetic electrons with a small angular spread produced in a dedicated photoelectron source (e gun) [37] located at the RS. These electrons span a 50 eV wide range of surplus energies E - qU and pass through the integral column density  $\rho d$  of the source. This allows us to measure the characteristics of single (s = 1) and multiple (s = 2, 3, ...)inelastic scattering in  $T_2$ . In Fig. 2 (top), we display the measured response f(E-qU) for a narrow-angle photoelectron source as well as the calculated response  $f_{\text{calc}}(E-qU)$  for isotropically emitted  $\beta$ -decay electrons for the normal integrating MAC-E mode for  $\rho d \approx \rho d_{\text{nom}}$ . The sharp rise with the filter width  $\Delta E$  to a plateau extending up to 11 eV results from "no loss" (energy loss  $\delta E = 0$ ) e-gun electrons, which leave the source without scattering (s = 0) with a probability  $\exp(-\rho d \cdot \sigma)$ . At larger E - qU, s-fold scattering (s = 1, 2, 3) is visible. In Fig. 2 (bottom), the differential data from the MAC-E-TOF mode [38] are shown, where the electron time of flight (TOF) is recorded. This allows us to even better assess the s-fold inelastic scattering and to obtain the energy-loss function of electrons  $\varepsilon(\delta E)$  by a deconvolution with the no loss peak at  $\delta E = E - qU = 0$ .

As the background rate  $R_{bg}$  exceeds its design goal of 0.01 counts per second (cps), we have studied the nature and origin of background processes so as to implement



FIG. 2. (top) Measured and calculated response functions f(E - qU) for electron surplus energies E - qU at different  $\rho d$  values of  $T_2$ . Measured f(E - qU) for a narrow-angle photoelectron source close to  $\rho d_{nom}$  and fit (cyan line); and calculated  $f_{calc}(E - qU)$  for isotropically emitted  $\beta$  decay electrons up to  $\theta_{max}$  at  $\rho d_{exp}$  (1.11 × 10<sup>17</sup> cm<sup>-2</sup>), the set point of our scans (red line), and in the limit of vanishing  $\rho d = 0$  (grey, dashed-dotted line). (bottom) Differential distributions of energy losses  $\delta E$  from the MAC-E-TOF mode after a selection 35  $\mu s \leq$  TOF  $\leq 50 \ \mu s$  at  $\rho d \approx \rho d_{nom}$  and fit (cyan line). The "no loss" peak at  $\delta E = E - qU = 0$  is followed by peaks with s = 2 (s = 3) scattering at twice (triple) the  $\delta E$  value of s = 1. The energy loss function  $\varepsilon(\delta E)$  for s = 1 is obtained by deconvolution (orange line).

mitigation measures. Up to now, source-related backgrounds have not been observed, so that spectrometerrelated processes [39] dominate  $R_{bg}$  apart from a small detector-related contribution [32]. Electrons generated at the spectrometer surface by cosmic muons and environmental gamma rays are inhibited from entering the inner flux tube by magnetic and electric barriers [40,41]. Thus,  $R_{bg}$  originates from excited or unstable neutral atoms which can propagate freely in the UHV environment. Accordingly,  $R_{bg}$  is observed to have an almost constant rate per unit volume in the flux tube.

Detailed investigations of the background behavior [39,42] revealed that a significant part of  $R_{bg}$  is due to Rydberg atoms sputtered off the inner spectrometer surfaces by <sup>206</sup>Pb-recoil ions following  $\alpha$  decays of <sup>210</sup>Po. These processes follow the decay chain of the long-lived <sup>222</sup>Rn progeny <sup>210</sup>Pb, which was surface-implanted from ambient air (activity  $\approx 1$  Bq/m<sup>2</sup>) during the construction phase. A small fraction of these Rydberg states is ionized by blackbody radiation when propagating over the magnetic flux tube. The resulting sub-eV scale electrons are accelerated to qU by the MAC-E-filter and form a Poisson component to  $R_{bg}$ .

The other part of background events stems from  $\alpha$  decays of single <sup>219</sup>Rn atoms ( $t_{1/2} = 3.96$  s) emanating from the

NEG pumps located in two of the three pump ports of the main spectrometer which release a large number of electrons up to the keV scale in the flux tube, where they are stored due to its magnetic bottle characteristics. By scattering off residual gas, the stored electrons subsequently produce secondary background electrons. This process continues until the stored electron is cooled off to an energy of a few eV when it can escape and also contribute itself to  $R_{bg}$  at qU. Owing to its origin from a small number of <sup>219</sup>Rn decays, this background results in extended time periods where the background level is enhanced yielding a small non-Poissonian component [43]. Liquid-nitrogen cooled copper baffles at the inlet of the NEG pumps act as a countermeasure [44]. The coverage of the inner surface of the main spectrometer with a monolayer of  $H_2O$ , originating from an imperfect bake out of the prespectrometer, has led to the formation of a thin layer of H<sub>2</sub>O covering the baffle surface. Therefore, the retention of <sup>219</sup>Rn in this work is hampered such that  $R_{\rm bg}$ retains a small non-Poissonian component.

Measurements of the tritium  $\beta$  spectrum.—In the following, we report on our first high-purity tritium campaign from April 10 to May 13, 2019 which demonstrates the functionality of all system components and of the extensive tritium infrastructure at large source activity (2.45 × 10<sup>10</sup> Bq) and tritium throughput (4.9 g/day). As a result of radiochemical reactions of  $T_2$  with the previously unexposed inner metal surface of the injection capillary, we observe drifts in the source column density. To limit these drifts to a level of  $\pm 2 \times 10^{-2}$  over our campaign, we keep the column density at an average value of  $\rho d_{exp} = 1.11 \times 10^{17}$  molecules cm<sup>-2</sup>, which is about a factor of 5 smaller than  $\rho d_{nom}$ .

At this setting, the smaller value of  $\rho d_{exp} \cdot \sigma$  (0.404) reduces the amount of inelastic scattering of electrons off neutral gas, see Fig. 2. The relative fractions of the six hydrogen isotopologues injected into the source are continuously monitored by laser-Raman spectroscopy with  $10^{-3}$  precision [45]. The average isotopic tritium purity  $\varepsilon_T$ (0.976) of our analyzed data sample is derived from the composition of the tritiated species  $T_2$  (0.953), HT (0.035), and DT (0.011), with inactive species (D<sub>2</sub>, HD, and H<sub>2</sub>) being present only in trace amounts.

Because of the large number of  $\beta$  decay s and ionization processes, a cold magnetized plasma of electrons (meV to keV scale) and ions (meV scale) is formed which interacts with the neutral gas. The strong solenoidal field B<sub>WGTS</sub> and the resulting large longitudinal conductance of the plasma allow the coupling of its potential to the surface of the rear wall (RW) located at the RS and, thus, to control the starting energies of  $\beta$ -decay electrons over the volume [46]. Biasing the gold-plated RW disk with small areal variation of the work function to -0.15 V relative to the grounded beam tube gives a very good radial homogeneity of the source potential. This is verified during initial tritium scans

TABLE I.	$1\sigma$ systematic	uncertainties	$(\sigma_{\rm syst})$	for	$m_{\nu}^2$	in	eV <sup>2</sup> ,
averaged ov	er positive and	negative error	rs, usin	g th	e me	etho	od of
MC propaga	ation.						

Effect	Relative uncertainty	$\sigma(m_{\nu}^2)$ in eV <sup>2</sup>
Source properties		
$\rho d \cdot \sigma$	0.85%	0.05
Energy loss $\varepsilon(\delta E)$	$\mathcal{O}(1\%)$	Negligible
Beamline		0.05
B <sub>WGTS</sub>	2.5%	
B <sub>min</sub>	1%	
B <sub>max</sub>	0.2%	
Final state distribution	$\mathcal{O}(1\%)$	0.02
Fluctuations in scan k		0.05
HV stacking	2 ppm	
$\rho d$ variation	0.8%	
Isotopologue fractions	0.2%	
Background		
Background slope	1.7%/keV	0.07
Non-Poisson background	6.4%	0.30
Total syst. uncertainty		0.32

with fits of  $E_0$  over detector pixel rings, which do not show a significant radial variation.

Additional information on plasma effects is provided by comparing the line shape and position of quasimonoenergetic conversion electrons ( $L_3$ -32) from <sup>83 m</sup>Kr runs in  $T_2$  to <sup>83 m</sup>Kr runs without the carrier gas at 100 K [47]. We do not identify sizeable shifts (< 0.04 eV) or broadening (< 0.08 eV) of lines so that the contribution of plasma effects at  $\rho d_{exp}$  to the systematic error budget in Table I can be neglected.

The integral tritium  $\beta$ -decay spectrum is scanned repeatedly in a range from  $[E_0 - 90 \text{ eV}, E_0 + 50 \text{ eV}]$  by applying a set of nonequidistant HV settings to the inner electrode system. Each scan over this range takes a net time of about 2 h and is performed in alternating upward and downward directions to compensate for any timedependent drift of the system to first order. At each HV set point, the transmitted electrons are counted over time intervals varying from 17 to 576 s with typical values of ~300 s for points close to  $E_0$ . When setting a new HV value, we make use of a custom-made postregulation system for voltage stabilization and elimination of highfrequency noise. At the same time, a custom-made HV divider [48] continuously monitors the retarding voltage with ppm precision.

To limit the influence of systematic uncertainties for this Letter, we analyze a scan range covering the region of 40 eV below  $E_0$  (22 HV set points) and 50 eV above (5 HV set points). The nonuniform measuring time distribution in this interval is shown in Fig. 3(c). It maximizes the sensitivity for  $m_{\nu}^2$  by focusing on the narrow region below  $E_0$ , where the imprint of the neutrino mass on the spectrum is most pronounced [20]. Shorter time intervals with a set



FIG. 3. (a) Spectrum of electrons  $R(\langle qU \rangle)$  over a 90 eV-wide interval from all 274 tritium scans and best-fit model  $R_{calc}(\langle qU \rangle)$ (line). The integral  $\beta$  decay spectrum extends up to  $E_0$  on top of a flat background  $R_{bg}$ . Experimental data are stacked at the average value  $\langle qU \rangle_l$  of each HV set point and are displayed with  $1\sigma$ statistical uncertainties enlarged by a factor of 50. (b) Residuals of  $R(\langle qU \rangle)$  relative to the  $1\sigma$  uncertainty band of the best fit model. (c) Integral measurement time distribution of all 27 HV set points.

point 200 V below  $E_0$  are interspersed to monitor the source activity, in addition to other measures [49].

Data analysis.—For each tritium scan with its 27 HV set points, we apply quality cuts to relevant slow-control parameters to select a data set with stable run conditions. This results in 274 scans with an overall scanning time of 521.7 h. We also define a list of 117 detector pixels (out of 148), which excludes those pixels that are noisy or shadowed by beam line instrumentation in the  $\beta$ -electron path along the magnetic flux tube. For the digitized, calibrated and pile-up-corrected detector spectra, a broad region of interest (ROI) between 14 and 32 keV is defined. The ROI takes into account the detector energy resolution and its elevated potential (+10 kV) and allows us to include a large fraction of electrons backscattered at the detector in the narrow scan region close to  $E_0$  resulting in a negligible contribution to the systematic uncertainty budget [32].

The long-term stability of the scanning process is verified by fits to single scans to extract their effective  $\beta$ -decay end points. The 274 fit values show no timedependent behavior and follow a Gaussian distribution ( $\sigma = 0.25$  eV) around a mean value of  $E_0 = 18573.7$  eV. In view of this and the very good overall stability of the slow-control parameters for our data set, we merge the data of all 274 scans over all 117 pixels into one single 90-eVwide spectrum, which is displayed in Fig. 3(a) in units of cps.

The underlying process corresponds to the "stacking" of events at the mean HV set points  $\langle qU \rangle_l$  (l = 1-27). The small Gaussian spread (rms = 34 mV) of the actual HV value  $qU_{l,k}$  during a scan k relative to  $\langle qU \rangle_l$ , the average of all scans, is a minor systematic effect which is accounted for in the analysis. The resulting stacked integral spectrum,  $R(\langle qU \rangle)$ , comprises  $2.03 \times 10^6$  events, with  $1.48 \times 10^6 \beta$ decay electrons below  $E_0$  and a flat background ensemble of  $0.55 \times 10^6$  events in the 90 eV scan interval. This highstatistics data set allows us to show  $1\sigma$  error bars enlarged by a factor of 50 in Fig. 3.

The experimental spectrum is well described by our detailed model of the KATRIN response to  $\beta$ -decay electrons and background. It contains four free parameters: the signal amplitude  $A_s$ , the effective  $\beta$ -decay end point  $E_0$ , the background rate  $R_{bg}$ , and the neutrino mass square  $m_{\nu}^2$ . We leave  $E_0$  and  $A_s$  unconstrained, which is equivalent to a "shape-only" fit. The goodness-of-fit is illustrated in Fig. 3(b) from the scatter of residuals around the error band of the model.

The four-parameter fit procedure over the averaged HV set points  $\langle qU \rangle_l$  compares the experimental spectrum  $R(\langle qU \rangle)$  to the model  $R_{calc}(\langle qU \rangle)$ . The latter is the convolution of the differential  $\beta$ -electron spectrum  $R_{\beta}(E)$  with the calculated response function  $f_{calc}(E - \langle qU \rangle)$ , with an added energy-independent background rate  $R_{bg}$ 

$$R_{\text{calc}}(\langle qU \rangle) = A_s N_T \int R_{\beta}(E) f_{\text{calc}}(E - \langle qU \rangle) dE + R_{\text{bg}}.$$
(1)

Here,  $N_T$  denotes the calculated number of tritium atoms in the source multiplied with the accepted solid angle of the setup  $\Delta\Omega/4\pi = (1 - \cos\theta_{\rm max})/2$  and the detector efficiency  $[\theta_{\rm max} = \arcsin\sqrt{(B_{\rm WGTS}/B_{\rm max})} = 50.4^{\circ}]$ , its uncertainty is absorbed by the fit parameter  $A_s$ .

The electron spectrum  $R_{\beta}(E)$  from the superallowed  $\beta$  decay of molecular tritium is calculated using Fermi's Golden Rule

$$R_{\beta}(E) = \frac{G_F^2 \cdot \cos^2 \Theta_C}{2\pi^3} |M_{\text{nucl}}^2| F(E, Z') \\ \times (E + m_e) \sqrt{(E + m_e)^2 - m_e^2} \\ \times \sum_j \zeta_j \varepsilon_j \sqrt{\varepsilon_j^2 - m_\nu^2} \Theta(\varepsilon_j - m_\nu), \qquad (2)$$

with the square of the energy-independent nuclear matrix element  $|M_{nucl}^2|$ , the Fermi constant  $G_F$ , the Cabibbo angle  $\Theta_C$ , the electron mass  $m_e$ , the Fermi function F(E, Z' = 2), and the neutrino energy  $\varepsilon_j = E_0 - E - V_j$ . In addition, our

calculations incorporate radiative corrections (for details, see [12,20]), and we account for thermal Doppler broadening at 30 K.

When calculating  $R_{\beta}(E)$ , we sum over a final-state distribution (FSD) which is given by the probabilities  $\zeta_i$ with which the daughter ion  ${}^{3}\text{He}T^{+}$  is left in a molecular (i.e., a rotational, vibrational, and electronic) state with excitation energy  $V_i$ . For this analysis, we first confirm the most recent theoretical FSD calculations [50,51] using new codes for solving the electronic and rovibrational problems within the Born-Oppenheimer approximation. We then refine the FSD by adopting a more efficient treatment of the rovibrational part and an update of other kinematicsrelated quantities, such as molecular masses, as well as recoil parameters (momenta and kinetic energy shifts). Most importantly, we treat all isotopologues  $(T_2, HT, and$ DT) in a consistent way with initial angular momenta distributions  $J_{\kappa}$  ( $\kappa = 0, ..., 3$ ) at 30 K for the electronic bound states n = 1, ..., 6. The FSD includes higher excitation energies up to the continuum based on [50], but their contribution to our analysis interval  $[E_0 - 40 \text{ eV}]$  is at an overall level of 10<sup>-4</sup> only. Accordingly, the FSD uncertainties in our narrow analysis interval of 40 eV below  $E_0$ only contribute at the level of  $0.02 \text{ eV}^2$  to the total systematics budget on  $m_{\nu}^2$  (see Table I).

The response function  $f_{calc}(E - qU)$  used in the analysis is shown as the red curve in Fig. 2 (top). It corresponds to  $\beta$ -decay electrons born with energies close to  $E_0$  and emitted isotropically up to  $\theta_{max}$  in the source gas. Compared to the *e*-gun beam, they possess a different distribution of energy losses due to their broader range of pitch angles  $\theta$  and the varying amount of source gas ( $\rho d$ ) they traverse. These processes are studied on the basis of gas dynamical simulations [52] which yield an approximately triangular-shaped longitudinal source profile.

After modeling the energy loss of  $\beta$ -decay electrons through the source by making use of  $\rho d \cdot \sigma$  and  $\varepsilon(\delta E)$ , their subsequent propagation is tracked by the KASSIOPEIA simulation software [53]. It incorporates a detailed beam line model which takes account of the small radial inhomogeneities of  $B_{\min}$  and qU at the analyzing plane. The full model provides the detailed shape of  $\Delta E$  and the distribution of electron pitch angles up to  $\theta_{\max}$  from the parameters of the magnetic field triplet ( $B_{WGTS}$ ,  $B_{\min}$ ,  $B_{\max}$ ).

The energy-independent part of  $R_{\text{calc}}(\langle qU \rangle)$ ,  $R_{\text{bg}}$ , comes from a fit of the spectrum  $R(\langle qU \rangle)$  over our 90 eV scan range. The fit value  $R_{\text{bg}} = (0.293 \pm 0.001)$  cps is largely constrained by the 5 HV set points above  $E_0$  and agrees with data from independent background runs taken with an empty source before the tritium measurements.

The resulting model,  $R_{\text{calc}}(\langle qU \rangle)$ , is then fitted to  $R(\langle qU \rangle)$ . To ensure that this proceeds without bias, we employ a twofold "blinding" scheme. The first blinding step leaves the data untouched, but a modification is

applied during the building of the model  $R_{\text{calc}}(\langle qU \rangle)$ . The FSD part describing rovibrational excitations of the electronic ground state is replaced with a Gaussian distribution with parameters not accessible to the analysis at first. As a result, fits with the blinded FSD do not reveal the unbiased value of  $m_{\nu}^2$ . The "true" FSD is revealed only at the last step ("unblinding") after having fixed all model inputs and systematic uncertainties.

The second measure to mitigate biasing is to perform the full analysis, including parameter fitting, using Monte Carlo–based (MC) data sets first, before turning to the experimental data. For each experimental scan k, we generate a "MC twin,"  $R_{calc}(\langle qU \rangle)_k$ , from its averaged slow-control parameters to procure  $R_\beta(E)_k$ ,  $f_{calc}(E-\langle qU \rangle)_k$ , and  $R_{bg,k}$ . Analysis of MC twins allows us to verify the accuracy of our parameter inference by recovering the correct input MC values for  $m_\nu^2$ . This approach is also used to assess statistical ( $\sigma_{stat}$ ) and systematic ( $\sigma_{syst}$ ) uncertainties and to compute our expected sensitivity.

In the following, we report on the results of two independent analyses with different strategies to propagate systematic uncertainties: the "Covariance Matrix" and the "MC propagation" approaches.

In the covariance method, we fit the experimental spectrum  $R(\langle qU \rangle)$  with the model  $R_{\text{calc}}(\langle qU \rangle)$  by minimizing the standard  $\chi^2$  estimator. To propagate the systematic uncertainties, a covariance matrix is computed after performing  $O(10^4)$  simulations of  $R_{\text{calc}}(\langle qU \rangle)$ , while varying the relevant parameters for each calculation according to the likelihood given by their uncertainties [35,54,55]. The resulting systematic uncertainties agree with the values shown in Table I, which is based on the second approach. The sum of all matrices encodes the total uncertainties of  $R_{\text{calc}}(\langle qU \rangle)$  and their HV set point dependent correlations. The  $\chi^2$  estimator is then minimized to determine the four best-fit parameters, and the shape of  $\chi^2$  function is used to infer the uncertainties. The results of this fit are displayed in Fig. 3. We obtain a goodness-of-fit of  $\chi^2 = 21.4$  for 23 d.o.f., corresponding to a p value of 0.56.

The MC-propagation approach is a hybrid Bayesianfrequentist method, adapted from Refs. [56–58]. We fit the experimental spectrum  $R(\langle qU \rangle)$  with the model  $R_{calc}(\langle qU \rangle)$  by minimizing the negative Poisson-likelihood function. The goodness-of-fit of  $-2 \ln \mathcal{L} = 23.3$  for 23 d.o.f. corresponds to a *p* value of 0.44. To propagate the systematic uncertainties, we repeat the fit 10<sup>5</sup> times, while varying the relevant parameters in each fit according to their uncertainties given in column 2 of Table I.

We report the  $1\sigma$  width of the fit parameters as their systematic uncertainty in the third column of Table I. In order to simultaneously treat statistical and all systematic uncertainties, each of the  $10^5$  fits is performed on a statistically fluctuated MC copy of the true data set, leading to the distributions of  $m_{\nu}^2$  and  $E_0$  shown in Fig. 4.



FIG. 4. Scatter plot of fit values for the mass square  $m_{\nu}^2$  and the effective  $\beta$ -decay end point  $E_0$  together with  $1\sigma$  (black) and  $2\sigma$  (blue) error contours around the best fit point (cross). It follows from a large set of pseudoexperiments emulating our experimental data set and its statistical and systematical uncertainties.

The strong correlation (0.97) between the two parameters is an expected feature in kinematic studies of  $\beta$  decay [11,12]. The final-best fit is given by the mode of the fit-parameter distributions, and the  $1\sigma$  total error is determined by integrating the distributions up to 16% from either side.

*Results.*—The two independent methods agree to within a few percent of the total uncertainty. As best fit value for the neutrino mass, we find  $m_{\nu}^2 = (-1.0^{+0.9}_{-1.1}) \text{ eV}^2$ . This best fit result corresponds to a  $1\sigma$  statistical fluctuation to negative values of  $m_{\nu}^2$  possessing a *p* value of 0.16.

The total uncertainty budget of  $m_{\nu}^2$  is largely dominated by  $\sigma_{\text{stat}}$  (0.97 eV<sup>2</sup>) as compared to  $\sigma_{\text{syst}}$  (0.32 eV<sup>2</sup>). As displayed in Table I, the dominant contributions to  $\sigma_{\text{syst}}$  are found to be the non-Poissonian background from radon and the uncertainty on the background slope, which is constrained from the wide-energy integral scans of the earlier "first tritium" data [35]. Uncertainties of the column density, energy-loss function, final-state distribution, and magnetic fields play a minor role in the budget of  $\sigma_{\text{syst}}$ . Likewise, the uncertainties induced via fluctuations of  $\varepsilon_T$ and HV parameters during a scan are negligibly small compared to  $\sigma_{\text{stat}}$ . The statistical (systematic) uncertainty of our first result on  $m_{\nu}^2$  is smaller by a factor of 2 (6) compared to the final results of Troitsk and Mainz [24,25].

The methods of Lokhov and Tkachov (LT) [59] and of Feldman and Cousins (FC) [60] are then used to calculate the upper limit on  $m_{\nu}$ . Both procedures avoid empty confidence intervals for nonphysical negative best-fit estimates of  $m_{\nu}^2$ . For this first result, we follow the LT method. For a statistical fluctuation into the nonphysical region the method returns a confidence belt that coincides with the experimental sensitivity and avoids a shrinking upper limit for more negative values of  $m_{\nu}^2$ . Using the LT construction, we derive an upper limit of  $m_{\nu} < 1.1$  eV (90% C.L.) as the central result of this Letter. By construction, it is identical to the expected sensitivity. For completeness, we also note the FC upper limits  $m_{\nu} < 0.8(0.9)$  eV at 90% (95%) C.L.

For the effective end point, our two analysis methods both obtain the best-fit value  $E_0 = (18573.7 \pm 0.1) \text{ eV}$ (see Fig. 4). At this level of precision, a consistency check on the energy scale of KATRIN can be performed by comparing our experimental Q value for molecular tritium with that based on measurements of the <sup>3</sup>He-<sup>3</sup>H atomic mass difference [61]. Our result for the Q value of  $(18575.2 \pm 0.5)$  eV is obtained from our best-fit value for  $E_0$  by adding the center-of-mass molecular recoil of  $T_2$  (1.72 eV) [11], as well as the relative offset  $(-0.2 \pm 0.5 \text{ eV})$  of the source potential to the work function of the inner electrode. The calculated Q value from the  ${}^{3}\text{He-}{}^{3}\text{H}$  atomic mass difference is (18575.72  $\pm$ 0.07) eV when accounting for the different binding energies and kinematic variables of atomic and molecular tritium [11]. The consistency of both Q values underlines the robustness of the energy scale in our scanning process of molecular tritium.

Conclusion and outlook.—The reported upper limit  $m_{\nu} < 1.1$  eV (90% C.L.) improves upon previous results [24,25] by almost a factor of 2 after a measuring period of only four weeks while operating at reduced column density. It is based on a purely kinematic method. As such, it has implications for both particle physics and cosmology. For the former, it narrows down the allowed range of quasidegenerate neutrino mass models by a direct method. For the latter, this model-independent limit can be used as laboratory-based input for studies of structure evolution in ACDM and other cosmological models.

Our result shows the potential of KATRIN to probe  $m_{\nu}$  by a direct kinematic method. After 1000 days of data taking at nominal column density and further reductions of systematics and  $R_{\rm bg}$ , we will reach a sensitivity of 0.2 eV (90% C.L.) on  $m_{\nu}$ , augmented by searches for physics beyond the SM, such as for sterile neutrino admixtures with masses from the eV to the keV scale.

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