

Chapter 2

The KATRIN Experiment

This chapter gives an overview of tritium β -decay experiments, introduces the Karlsruhe Tritium Neutrino Experiment (KATRIN) which is targeted to measure the neutrino mass with a sensitivity of $200 \text{ meV}/c^2$, and finally outlines the motivation of this thesis. The chapter is structured as follows: Sect. 2.1 briefly describes the physics of tritium β -decay and the principle of a MAC-E-Filter. The section ends with a view back on previous neutrino experiments. In Sect. 2.2 the requirements of the KATRIN experiment are discussed and an overview of its main components is given. Then, a deeper insight into the physical properties of the windowless gaseous tritium source is given in Sect. 2.3 and the implications for control and monitoring of this most complex KATRIN component are deduced. Finally, Sect. 2.4 focuses on the requirements for the laser Raman system of KATRIN, which imply that an accurate calibration of this system is required in order to stay within the stringent budget of systematic uncertainties so that KATRIN can reach its design sensitivity.

The main references for this chapter are the Technical Design Report of KATRIN [30] and a recent review paper [13].

2.1 Tritium β -decay Experiments

Up to the date of the compilation of this thesis, the most sensitive direct searches for the neutrino mass are based on the tritium β -decay and the investigation of the energy spectrum of β -electrons close to the kinematic endpoint [13].

2.1.1 Tritium β -decay and the Neutrino Mass

The super-heavy hydrogen isotope tritium (T) is unstable and decays according to the following reaction into a daughter nucleus via the emission of a pair of leptons, an electron, and an electronanti-neutrino:

$$\text{T} \rightarrow {}^3\text{He}^+ + \text{e}^- + \bar{\nu}_e. \quad (2.1)$$

In 1934, Enrico Fermi published a fundamental theory of β -decay [17], based on the neutrino hypothesis by Wolfgang Pauli in 1930 (the relevant letters and publications are summarized in [45]). This theory allows to derive essential features of the decay, and also serves to derive an expression of the β -electron spectrum which is used in the analysis of the neutrino mass.

The calculation of the electron energy spectrum starts with Fermi's famous Golden rule

$$\frac{dN}{dt} = \frac{2\pi}{\hbar} |M^2| \rho. \quad (2.2)$$

M is the transition matrix element and ρ describes the density of final states. In principle, Eq. 2.2 needs to be integrated over all possible discrete and continuous final states.

The derivation results¹ in the following expression for the differential decay rate as function of the energy ($\dot{N}(E) = d^2N/(dt dE)$)

$$\begin{aligned} \dot{N}(E) = & C \cdot F(E, Z + 1) \cdot (E + m_e c^2) \cdot \sqrt{(E + m_e c^2)^2 - m_e^2 c^4} \\ & \cdot (E_0 - E) \cdot \sqrt{(E_0 - E)^2 - m(\nu_e)^2 c^4} \cdot \Theta(E_0 - E - m(\nu_e) c^2). \end{aligned} \quad (2.3)$$

The kinetic energy and the rest mass of the electron are denoted by E and m_e , respectively. The endpoint energy E_0 of the electrons (=maximum kinetic energy) is given by the reaction energy, Q , and the recoil energy² of the ${}^3\text{He}^+$ nucleus, E_{rec} : $E_0 = Q - E_{\text{rec}}$ assuming $m(\nu_e) = 0$. The Fermi function, $F(E, Z + 1)$, takes into account the Coulomb interaction of the emitted β -electron and the daughter nucleus with charge $Z + 1$ [26]. The Heaviside step function $\Theta(\dots)$ ensures conservation of energy.

Note that the β -decay of tritium is of the superallowed type which implies that the nuclear matrix element M_{nuc} is energy independent [44]. Accordingly, it can be contracted in the constant C

$$C = \frac{G_F^2 \cdot \cos^2 \theta_C}{2\pi^3 \hbar^7 c^5} \cdot |M_{\text{nuc}}^2|. \quad (2.4)$$

with Fermi's coupling constant G_F and θ_C denoting the Cabbibo angle.

The formula given in Eq. 2.3 is an approximation only, and therefore will be extended with regard to two important aspects for high-resolution β -spectroscopy. First, as discussed in the introduction chapter, the neutrino mass $m(\nu_e)$ is treated as a superposition of three mass eigenstates $m(\nu_i)$ as stated in Eq. 1.44. As will

¹ The reader is referred to [13, 44], and [67] for the full derivation.

² The variation of the recoil energy in the endpoint region ($E_0 - 30 \text{ eV} \dots E_0$) amounts to only $\Delta E_{\text{rec}} = 3.5 \text{ meV}$, and therefore can be assumed as constant [41].

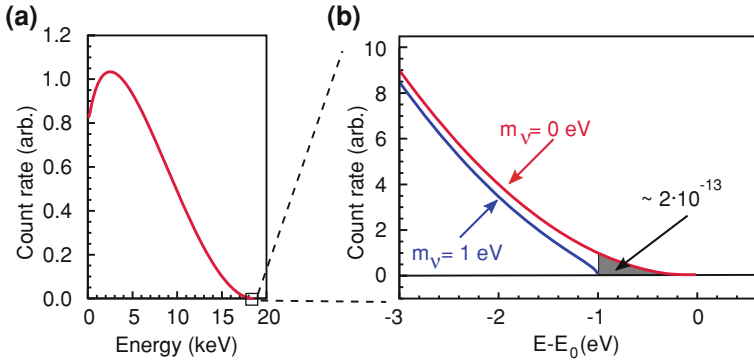


Fig. 2.1 The electron energy spectrum of tritium β -decay. **a** Full energy range, **b** Energy range around the kinematic endpoint of about $E_0 = 18.6$ keV. The spectrum is shown for two exemplary cases: (i) for a vanishing neutrino mass $m(\nu_e) = 0$ eV/ c^2 , and (ii) for a neutrino mass of $m(\nu_e) = 1$ eV/ c^2 . The shaded area represents only a fraction of 2×10^{-13} of all tritium β -decays

be shown below, the present experimental resolution does not allow to disentangle these mass states, so that an average mass is measured (c.f. Eq. 1.44). Second, all final states of the daughter system (atom or molecule³) with individual probabilities P_j and excitation energies V_j have to be accounted for. Thus each final state j has a corresponding specific endpoint $E_j = E_0 - V_j$. Both effects are integrated into Eq. 2.3 by a double summation.

This finally leads to following expression (slightly modified from [13])

$$\dot{N}(E) = C \cdot F(E, Z+1) \cdot (E + m_e c^2) \cdot \sqrt{(E + m_e c^2)^2 - m_e^2 c^4} \cdot \left(\sum_{i,j} |U_{ei}^2| \cdot P_j \cdot (E_j - E) \cdot \sqrt{(E_j - E)^2 - m(\nu_i)^2 c^4} \cdot \Theta(E_j - E - m(\nu_i) c^2) \right). \quad (2.5)$$

Figure 2.1 shows the overall energy spectrum of electrons from β -decay and a zoom into the endpoint region at about $E_0 = 18.6$ keV. The latter reveals the influence of a non-vanishing neutrino mass on the spectral shape. It underlines the generic fact that a finite neutrino mass leads to a shift of the spectral endpoint. Furthermore, the spectrum is distorted in an energy interval of several eV due to the extended momentum range where neutrinos are non-relativistic. The neutrino mass $m(\nu_e)$ can be obtained via fitting Eq. 2.5 to the measured data, while taking into account a variety of instrumental-related effects.

³ In the case of a decaying atom only electronic excitation need to be considered. Molecules also can be excited to vibrations and rotations.

2.1.2 The MAC-E-Filter Measurement Principle

The spectral shape close to the endpoint in Fig. 2.1 indicates two major issues when measuring the neutrino mass. First, a high energy resolution in the order of 1 eV is required to observe the mass-dependent transition of the energy-momentum relation of the emitted neutrino over a specific momentum range. Second, the tritium source has to provide a very high β -intensity since the emission probability of an electron in the region-of-interest is tiny. The respective β -decay count rate should be at least a factor of two higher than the rate of background events, calling for an almost background-free detection technique.

A technique which combines both features is based on the so-called MAC-E-Filter principle (Magnetic Adiabatic Collimation with an Electrostatic filter). This spectrometer type is based on the pioneering work of Kruit and Read [34], as well as of Beamson and co-workers [6]. It was further refined and adapted for neutrino mass measurements in Mainz [47] and Troitsk [38].

The main principle of the MAC-E-Filter is shown in Fig. 2.2. A tritium source and an electron detector are located each in a superconducting solenoid. The solenoids generate a magnetic guiding field for electrons from the β -source to the detector. During propagation, the electrons gyrate around the field lines in a cyclotron motion since their starting momentum is isotropic in general, and thus not parallel to the magnetic field lines. Their kinetic energy can be decomposed into a component $E_{\perp}$ transverse and a component $E_{\parallel}$ longitudinal to the magnetic field lines. The method of magnetic guidance allows for an accepted solid angle of about 2π , in principle.

The magnetic field, B , reaches its minimum value in the middle between both solenoids. At this plane the field strength is several orders of magnitudes lower than at the center of the solenoids. As the transition of the magnetic field to its minimum value and back again is adiabatic, in a non-relativistic approximation the magnetic moment of the electron μ is constant [27]

$$\mu = \frac{E_{\perp}}{B} = \text{const.} \quad (2.6)$$

The strong decrease of the magnetic field B thus leads to a reduction of the $E_{\perp}$ component by the same amount, in order to keep μ invariant. The transversal component is thus transformed by the magnet gradient force into the longitudinal direction due to the adiabaticity of this process, with a small transversal component remaining at the mid plane. When discussing the MAC-E-Filter principle, it is important to recall that the magnetic flux $\Phi = \mathbf{A} \cdot \mathbf{B}$ is conserved. This leads to an increase of the beam cross-sectional area A by the same factor as the magnetic field B drops. The final result is a broad beam of electrons flying nearly parallel to the field lines at the center of the MAC-E-Filter. This is called magnetic adiabatic collimation of the MAC-E-Filter.

The second part is related to the electrostatic filter. The analysis of the kinetic energy of the electrons is performed in the plane of lowest magnetic field and thus in the area where the transformation into longitudinal energy is maximal. Accordingly,

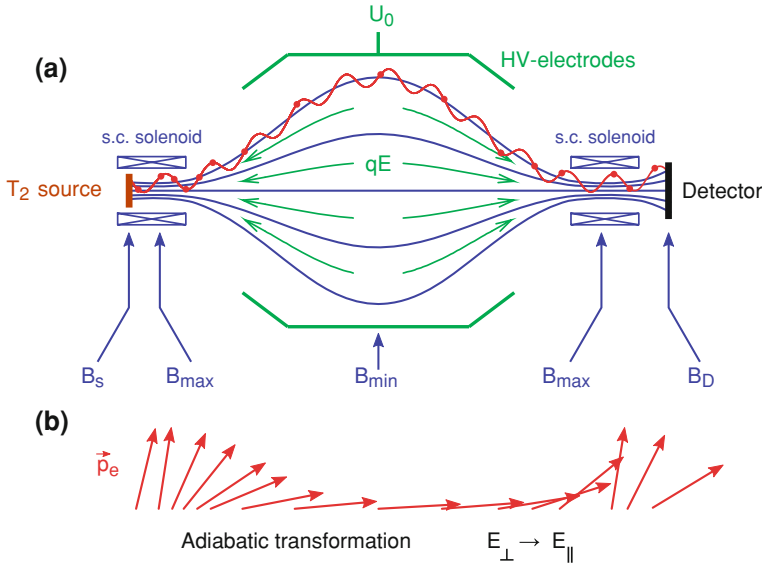


Fig. 2.2 Principle of the MAC-E-Filter. A detailed explanation is given in the main text. **a** An inhomogeneous magnetic field B is generated by a system of superconducting solenoids (blue). These solenoids magnetically guide β -decay electrons from the tritium source to the electron detector. The decrease of the magnetic field between solenoids (plane of energy analysis) increases the area of the field lines. The electric retardation field is generated in such way that it is parallel to the magnetic field lines. **b** The momentum is transformed by a gradient force due to the adiabatic invariance of the magnetic moment of the electron μ in the inhomogeneous B -field. The highest degree of parallelism is obtained in the central region of $B_{\min}$

an electrostatic barrier created by cylindrical electrodes allows to filter the electrons. The filter can only be passed by electrons with higher kinetic energy than the potential from the retardation voltage U_0 . This feature turns the MAC-E filter into a high pass filter. The adiabatic transformation into the longitudinal direction is of course imperfect by its very nature. For an isotropic β -source, the relative sharpness of the MAC-E-Filter is given by the ratio of the (minimal) magnetic field in the plane of energy analysis and the (maximal) field at the so-called pinch magnet which can be placed anywhere between source and detector

$$\frac{\Delta E}{E} = \frac{B_{\min}}{B_{\max}}. \quad (2.7)$$

At KATRIN, the plane of highest magnetic field $B_{\max}$ (at the pinch magnet) is located at the detector-facing side of the main spectrometer (see e.g. [20]) generating a field of 6 T. With a minimum field in the central spectrometer plane of 0.3 mT, a relative sharpness, $\Delta E/E$, of 1:20000 can be achieved. More details on the filter and its features are available in [8, 30, 47].

2.1.3 Results of Previous Neutrino Mass Experiments at Mainz and Troitsk

Two research groups have independently developed and operated MAC-E-Filters for the measurement of the neutrino mass from tritium β -decay up to now. The experiments were located at Mainz [47] and Troitsk [38] and mainly differed in the employed tritium sources which exhibit different systematic uncertainties.

At Mainz, the experiment included a MAC-E-Filter type spectrometer with a diameter of 1 m and a quench-condensed molecular tritium film as β -source operated at $T < 3$ K [9]. Several solid state effects like inelastic scattering of β -electrons in the T_2 film [2], the excitation of neighboring molecules [31] and self-charging [10] were identified as main systematic uncertainties. The analysis of the data set (the so-called Mainz phase II [33]) led to a resulting observable of

$$m(\nu_e)^2 = (-0.6 \pm 2.2_{\text{stat}} \pm 2.1_{\text{sys}}) \text{ eV}^2/\text{c}^4. \quad (2.8)$$

This can be translated, using the Feldman–Cousins method [16], into an upper limit for the neutrino mass of

$$m(\nu_e) < 2.3 \text{ eV}/\text{c}^2 \text{ (95 \% C.L.)}. \quad (2.9)$$

The Troitsk group employed a slightly larger spectrometer with 1.2 m in diameter and a windowless gaseous tritium source (WGTS) [7]. In 1999, a result was published which included an unexplained spectral anomaly near the endpoint [39]. Taking into account this distortion, an upper limit of $m(\nu_e) < 2.5 \text{ eV}/\text{c}^2$ (95 % C.L.) was reported.

In 2011, the group at Troitsk reanalysed their data from 1994–2004 with refined methods. Specifically, time-dependent effects in their WGTS and the selection of periods with good data stability and quality were carefully considered. This new analysis has resulted in [3]

$$m(\nu_e)^2 = (-0.67 \pm 1.89_{\text{stat}} \pm 1.68_{\text{sys}}) \text{ eV}^2/\text{c}^4, \quad (2.10)$$

which corresponds via Feldman–Cousins [16] to a new upper limit of

$$m(\nu_e) < 2.05 \text{ eV}/\text{c}^2 \text{ (95 \% C.L.)}. \quad (2.11)$$

2.2 The Karlsruhe Tritium Neutrino Experiment

The Karlsruhe Tritium Neutrino Experiment (KATRIN) is targeted to improve the current experimental sensitivity as obtained from Mainz and Troitsk from $2 \text{ eV}/\text{c}^2$ by a factor of ten to $200 \text{ meV}/\text{c}^2$ [30]. This major step in sensitivity can only be

achieved by substantially increasing the statistics and reducing systematic effects significantly at the same time.

2.2.1 Projected Sensitivity on Neutrino Mass

Detailed investigations reported in [30] have shown that the reference KATRIN setup will feature, after 3 years of measurements, a statistical uncertainty of the observable $m(\nu_e)^2$ of $\sigma_{\text{stat}} = 18 \times 10^{-3} \text{ eV}^2/\text{c}^4$. This value is of the same level as the total systematic uncertainty, which is anticipated to be $\sigma_{\text{sys,tot}} \leq 17 \times 10^{-3} \text{ eV}^2/\text{c}^4$. Both errors add up quadratically to the total uncertainty

$$\sigma_{\text{tot}} = \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{sys,tot}}^2} \approx 25 \times 10^{-3} \text{ eV}^2/\text{c}^4. \quad (2.12)$$

This would imply that a 5σ significance is given for discovering a neutrino mass of

$$m(\nu_e) = 350 \text{ meV}/\text{c}^2. \quad (2.13)$$

In case that no neutrino mass signal would be seen in the data, the total uncertainty can be translated into a new upper mass limit of

$$\begin{aligned} m(\nu_e) &\leq \sqrt{1.64 \cdot \sigma_{\text{tot}}} \\ &\leq 200 \text{ meV}/\text{c}^2 \text{ (90 \% C.L.)}. \end{aligned} \quad (2.14)$$

In order to reach this ambitious goal, the next-generation experiment KATRIN needs to be designed along the following requirements [30]:

- It is aimed to increase the signal rate at the endpoint of the β -spectrum by a factor of 100 compared to the predecessor experiments at Troitsk and Mainz. Further improvement of the statistics is achieved by a 10times longer measurement time (three “full-beam” years or, equivalently, five calendar years).
- The energy resolution of MAC-E-Filter type spectrometer should be $\Delta E < 1 \text{ eV}$ at 18.6 keV.
- The overall background rate measured at the electron detector should be $< 10^{-2} \text{ cps}$.
- All sources of systematic uncertainties of $m(\nu_e)^2$ need to be reduced by a factor of 100, so that statistical and systematic uncertainties are of similar size. The total systematic uncertainty budget $\sigma_{\text{sys,tot}} \leq 17 \times 10^{-3} \text{ eV}^2/\text{c}^4$ is composed of five main sources of uncertainties (see [13, 30]). Accordingly, the individual systematic uncertainties should not surpass the uncertainty budget of

$$\sigma_{\text{sys,ind}} \leq 7.5 \times 10^{-3} \text{ eV}^2/\text{c}^4. \quad (2.15)$$

The two sources of uncertainties from the tritium source which are directly related to this thesis are discussed in detail in Sect. 2.3.

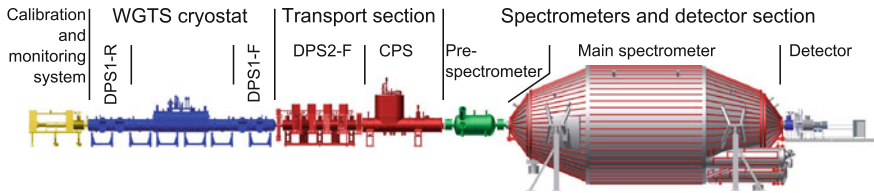


Fig. 2.3 Setup of the KATRIN experiment. For the explanation of the main components see text

2.2.2 Experimental Overview

The aforementioned requirements were considered and implemented in the design of the KATRIN experiment. A side view on the 70 m long setup is provided in Fig. 2.3. All relevant main components will be introduced in a compact way below. The reader is referred to the KATRIN design report [30] for further reading; additionally, recent publications or PhD theses which focus on specific sub-systems in more detail are cited at the end of each paragraph. Towards the end of this chapter, the focus is set on the windowless gaseous tritium source since this thesis is closely related to measuring important source properties.

The description is following the road of the electron from its point of origin in the source to its point of detection at the detector surface.

The Windowless Gaseous Tritium Source (WGTS) KATRIN will make use of a high luminosity gaseous molecular tritium source as pioneered by the Troitsk [7] and Los Alamos [53] groups. In Fig. 2.4 its conceptual design is visualized. Molecular tritium (5×10^{19} molecules/s) is injected in the middle of a stainless steel tube with a length of 10 m and a diameter of 90 mm. At both ends of the tube, tritium is pumped out at specific pump ports. This generates a longitudinal tritium density profile as sketched in the top panel of Fig. 2.4. The β -activity of the source is about 10^{11} electrons per second. The superconducting solenoid system surrounding the source tube guides the β -electrons adiabatically to the front and rear ends of source. The nominal magnetic field strength inside of the tube will be at 3.6 T. The WGTS is housed inside of a large and rather complex cryostat which is able to provide a stable temperature of the source tube at 30 K [22]. The WGTS is connected to the Inner Loop which provides a stable circulation of the gas through the source [60] and sustains the high tritium purity of the gas.

The key parameters of the WGTS as well as the extensive control and monitoring equipment are the focus of Sect. 2.3, where also the motivation for this thesis is found.

Further reading: [5, 60].

The transport system The two systems downstream of the WGTS forming the Source and Transport Section (STS) altogether are the Differential Pumping Section (DPS)⁴ and the Cryogenic Pumping Section (CPS). Their tasks are to magnetically

⁴ Note that the DPS1-F/R are part of the WGTS cryostat already, and the stand-alone system is called DPS2-F (see Fig. 2.3).

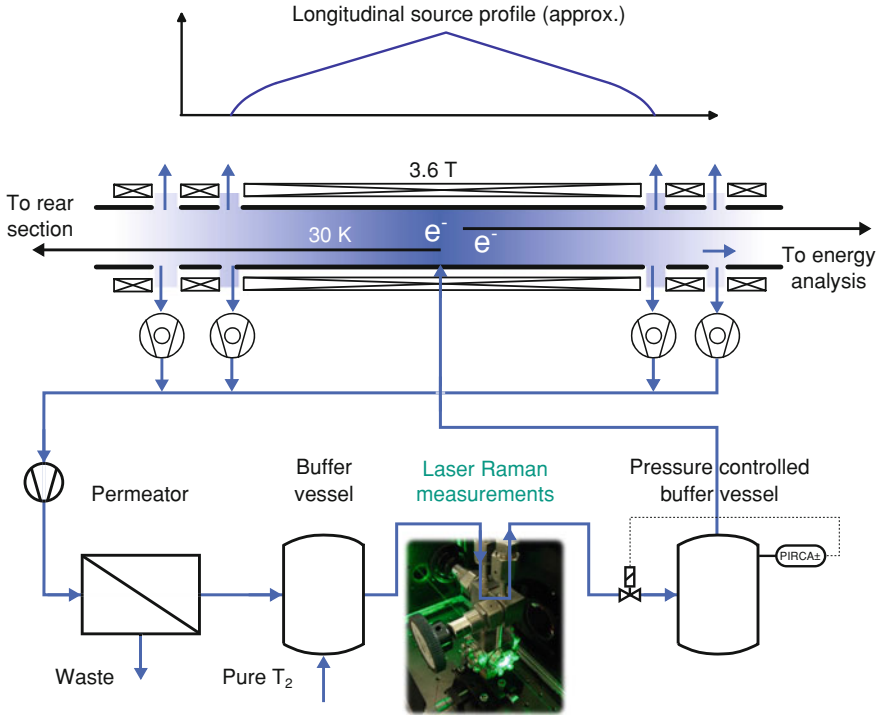


Fig. 2.4 Conceptual design of the Windowless Gaseous Tritium Source and Inner Loop. A stable tritium source profile (*top panel*) needs to be obtained during regular KATRIN operation. The density is highest at the injection point in the *middle* of the source tube and lowest at the pumping ports at the end of the tube. The gas circulation is provided by the Inner Loop [60]. Its parts are sketched in the *bottom* half of the figure. Pure tritium is obtained from the TLK infrastructure and filled into a buffer vessel. The composition of the gas is measured at a pressure of 100–200 mbar by a laser Raman system while it streams into the next buffer vessel. This vessel is pressure controlled and by this means it can provide a stable injection pressure which corresponds to a stable tritium flow rate (as long as the conductances of the injection capillary and the WGTS beam tube remain constant). The injected gas is pumped out by turbomolecular pumps and the return flow of the gas is then filtered from impurities by a permeator. This device consists of a PdAg membrane which is only permeable by hydrogen isotopologues (T_2 , DT, D_2 , HT, HD, and H_2); more details on permeators are given in Sect. 6.5.2. The impurities are handled by the TLK infrastructure and replaced by batches of “fresh” high-purity tritium

transport the electrons to the spectrometer section and further reduce the residual tritium which was not pumped out at the WGTS exit. These additional tritium retention systems are required to limit the amount of tritium entering the spectrometer. Decaying tritium within the spectrometer volume would lead to an elevated rate of background events [32, 43]. The tritium flow has to be reduced by 14 orders of magnitude by two very different techniques. The DPS actively removes tritium from the beam tube by turbomolecular pumps [40], while the CPS employs a passive cryosorption concept [21].

Further reading: [32].

The spectrometer system KATRIN employs a combination of two spectrometers of the MAC-E-Filter type. A pre-spectrometer (3.4 m length and 1.7 m diameter) is connected to the downstream end of the CPS marking the begin of the tritium-free area of the experiment where tritium levels are on a negligible level. This smaller-sized spectrometer offers the option of prefiltering, in which all electrons with kinetic energies of $E_0 - 300$ eV would be reflected so that only the electrons of highest energies enter the main spectrometer.

The task of the main spectrometer is to analyze the high-energy part of the β -decay electrons which carry information on the neutrino mass with an energy resolution of $\Delta E = 0.93$ eV at 18.6 keV (see Eq. 2.7). Several auxiliary systems provide highly accurate and stable control over the electrostatic retarding potential (e.g. see [15, 61, 62]) as well as on the magnetic fields (e.g. see [51, 66]) in the spectrometer.

Further reading: [20, 42, 48].

The Focal Plane Detector The detector at the end of the KATRIN beamline is a silicon-based PIN diode array with a detection efficiency of $>90\%$ [64]. It has been designed to count electrons which were transmitted through the MAC-E-Filters. It is highly segmented into a total of 148 pixels of the same area to obtain a spatial resolution over the entire transmitted flux tube of 191 Tcm^2 . This is of major importance for detecting inhomogeneities in the tritium source or spectrometer potentials. The system is at present close to being integrated with the main spectrometer for the extensive spectrometer commissioning phase starting in spring 2013.

Further reading: [24].

Calibration and monitoring system Upstream of the WGTS cryostat a calibration and monitoring system is located which has three major purposes: (i) It houses the rear-wall which will define the plasma potential relative to the spectrometer retarding voltage [5]; (ii) It measures the source activity via β -induced X-ray spectroscopy [50, 54]; and (iii) it provides an angular resolved electron gun [63] for the measurement of the column density of the molecular gas source via inelastic electron-gas scattering. At present the system has completed its conceptual design phase.

Further reading: [5].

Experimental location The KATRIN experiment has to cycle tens of grams of tritium per day through the WGTS. The official license for handling up to 40 g of the radioactive gas and the appropriate extensive infrastructure are available only at few places worldwide such as the Tritium Laboratory Karlsruhe (TLK) at the Karlsruhe Institute for Technology (KIT) [11, 46]. The TLK has set-up and operated a closed tritium cycle for storing, processing, and purifying of the various gases, and offers a research experience of 20 years. These conditions are unique in the civil tritium research and they make the TLK the perfect host facility for the KATRIN experiment. A view of TLK infrastructure units with their glove box structure is provided in Fig. 2.5.

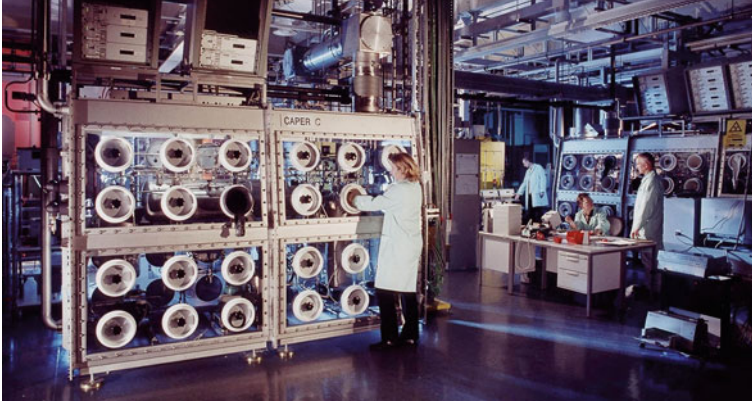


Fig. 2.5 View into the experimental hall of the Tritium Laboratory Karlsruhe (TLK). The person in the front works at a glove box which acts as secondary containment for the primary tritium system inside of it. This measure prevents contamination hazard for the workers and the laboratory

2.3 Properties of the WGTS

A gaseous molecular tritium source, which was employed in previous direct neutrino mass experiments (see [7] and [53]), is able to provide a high luminosity. This is of key relevance to achieve a high statistical sensitivity in the neutrino mass search. The essential parameters⁵ are the column density $\mathcal{N}$ and the isotopic composition (T_2 , DT , HT , D_2 , HD , H_2). The column density is defined as the number of molecules within the magnetic flux tube volume relative to the cross-sectional area in units of cm^{-1} . The activity $\mathcal{S}$ of the source is given as [5]

$$\mathcal{S} = C_S \cdot \epsilon_T \cdot \mathcal{N}. \quad (2.16)$$

where ϵ_T denotes the tritium purity and the proportionality constant C_S contains the experimental properties (acceptance angle, detector efficiency, ...).

For the determination of the neutrino mass it is important to control the two parameters, ϵ_T and $\mathcal{N}$, and to monitor their stability so that even tiny fluctuations can be accounted for in the off-line analysis.

2.3.1 Column Density

The gas column of the WGTS is built up and stabilized by the following approach [5] (see Fig. 2.4):

⁵ The nomenclature from the paper of Babutzka et al. [5] is employed here.

1. The gas is continuously injected into the middle of the source tube with an injection pressure p_{in} of about 10^{-3} mbar.
2. The gas streams to both ends of the central of the 10 m long and 90 mm wide beam tube, and it is pumped out there with constant pumping speed resulting in an outlet pressure p_{out} of about 1/20 of p_{in} .
3. The gas flow inside of the tube is governed by the viscosity of the gas which itself is a function of the temperature. For this reason the beam tube temperature has to be stabilized at a temperature region of about 30 K.

The stability of the column density of the WGTS is one of the major sources of systematic uncertainty at KATRIN [30]. In order to stay within the assigned uncertainty budget for the column density (see Eq. 2.15), it is required to obtain a precision of $\Delta_{\text{prec}}(\mathcal{N})/\mathcal{N} \leq 0.1\%$. Simulations have shown that it is necessary to stabilize p_{in} on the 0.1 % level, p_{out} to about 3 % and source tube temperature to better than 30 mK ($\pm 0.1\%$) [25, 30, 58].

The gas circulation is provided by the Inner Loop system sketched in Fig. 2.4 [60]. This closed loop system has been optimized to achieve a stable column density of $\mathcal{N} = 5 \times 10^{17}$ molecules per cm^2 . The observed stability of the injection pressure p_{in} in a test experiment surpassed the required 0.1 % by about an order of magnitude [49].

The WGTS is housed in a single more than 16 m long cryostat (see Fig. 2.6) which is able to provide a relative temperature stability of the source tube by a two-phase neon system [22]. The achieved stability at a WGTS mock-up named “Demonstrator” was $\Delta T = 1.5 \text{ mK h}^{-1}$ which is better than specified, too [23].

The column density, $\mathcal{N}$, is strongly related to the probability of inelastic scattering of the electrons off the source gas [37]. $\mathcal{N}$ is thus not only related to the β -rate, but also to energy losses, which distort the β -spectrum. For these reasons, the determination of N and the knowledge of the isotopic composition is of primary importance for KATRIN.

2.3.2 Isotopologue Composition

The other parameter which needs to be considered for the stability of the activity S in Eq. 2.16 is the tritium purity.

The tritium purity ϵ_{T} is given as the ratio of the number of tritium atoms to the total sum of atoms in the WGTS. The targeted purity value for the KATRIN measurement period is $\epsilon_{\text{T}} > 0.95$. This corresponds to a composition of about 90 % molecular tritium, T_2 , as the main gas constituent with a small admixture of DT (<10 %). The other hydrogen isotopologues (HT , D_2 , HD , and H_2) will be present as trace amounts only.

The stabilization of the gas composition is realized by connecting the Inner Loop to the tritium infrastructure of TLK as shown in Fig. 2.4. This interface allows extraction

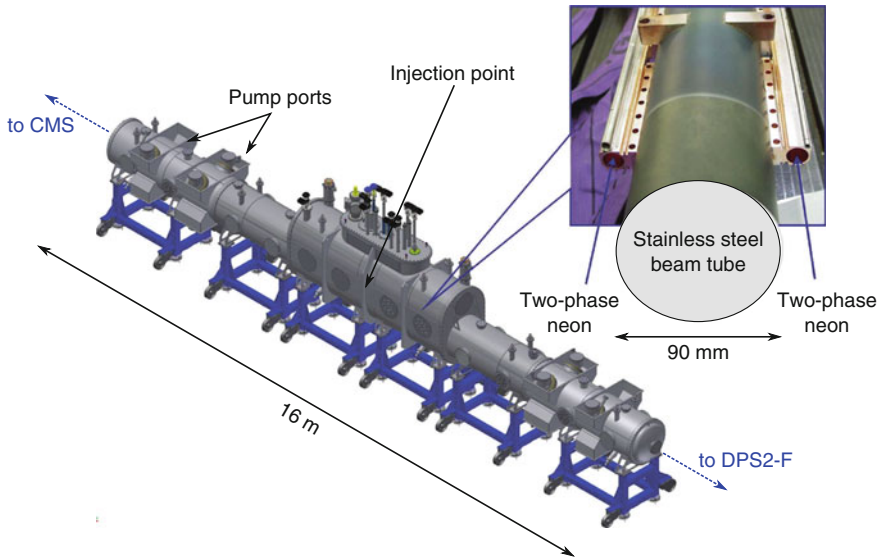


Fig. 2.6 Schematic view of the WGTS cryostat and beam tube cross-section. The ports for the turbomolecular pumps are indicated only at one end. The inlet shows the beam tube to which the two phase liquid neon cooling system is attached. Adapted from [13]

of parts of the impurities of the source gas and replacing them by (almost) pure tritium (up to 98 % [14]).

The monitoring of the gas composition is performed by a laser Raman system (LARA) which is integrated within the Inner Loop. Raman spectroscopy is an excellent instrument for the determination of the gas composition of the source gas. It is able to monitor all isotopologues simultaneously [59]. The principles of Raman spectroscopy and the experimental setup will be discussed in following chapters in detail, as they are closely related to the topic of this thesis.

The requirements on the accuracy of this system are discussed in the subsequent section.

2.4 Accuracy Requirements for the Monitoring of the Source Gas Composition

The accuracy of the monitoring system of the gas composition should be considered under two different aspects, which are precision and trueness.

Trueness is the fundamental quantity which describes the difference between the mean value of a measured observable and the true (reference) value. The precision is related to the square root of the statistical variance of several measured values around

their mean value. Thus, trueness is linked to systematic uncertainty, and precision to the statistical uncertainty [28].

A measurement can be called accurate if it is both, true and precise. A more detailed discussion of the two terms is found in Appendix A.

The KATRIN requirements for precision and trueness are discussed in the following.

Precision requirement The number of tritium atoms in the source governs the activity $\mathcal{S}$ of the source (see Eq. 2.16). Therefore, it is relevant to stabilize and monitor the tritium purity, ϵ_T , on the same 0.1 % precision level like the other parameters related to $\mathcal{N}$. By fulfilling this requirement it is possible to stay within the systematic uncertainty budget, $\sigma_{\text{sys,ind}}$, related to the tritium source.

Trueness requirement Until now, only relative changes of the gas composition were considered, which can be measured if the system's precision is sufficient. Trueness is not relevant at this point.

However, the composition of source gas is not only influencing the activity $\mathcal{S}$. Furthermore, non-negligible processes alter the β -electron energy and thus the shape of the β -spectrum. In general, the shape distortions are specific to each hydrogen isotopologue species involved. The relevant processes are summarized in the following list [30].

- **Nuclear recoil of the daughter molecule**

The momentum of the outgoing lepton pair is balanced by the daughter molecule ($^3\text{HeT}^+$, $^3\text{HeD}^+$, or $^3\text{HeH}^+$), which results in a specific recoil energy, E_{rec} . An approximation of this recoil energy for electron energies close to the endpoint, E_0 , is given by [30]

$$E_{\text{rec}} \approx E \cdot \frac{m_e}{m_{\text{daughter}}}. \quad (2.17)$$

The mass of the daughter molecule of the decay $\text{T}_2 \rightarrow ^3\text{HeT}^+$ is 1.5 times higher than of the decay $\text{HT} \rightarrow ^3\text{HeH}^+$. Thus, the recoil energy scales inversely: $E_{\text{rec}}^{\text{T}_2} = 1.72 \text{ eV}$ and $E_{\text{rec}}^{\text{HT}} = 2.58 \text{ eV}$, respectively [55]. As a result, the (unobserved) recoil energies of the different hydrogen isotopologues has to be taken into account on a statistical basis.

- **Doppler broadening**

The molecules in the source obey a thermal velocity according to the Maxwell-Boltzmann distribution [25] superimposed by a bulk velocity due to the diffusion of the molecules to both ends of the beam tube. Thus, the kinetic energy of the emitted electrons is affected by the quasi-stochastic movement of the decaying molecules. The non-relativistic approximation for the energy broadening of an

electron with $E \approx E_0$ emitted by a molecule flying parallel to the magnetic field lines is given by [30]

$$\Delta E = m_e \cdot |\mathbf{v}_e| \cdot |\mathbf{v}_{\text{mol}}|. \quad (2.18)$$

In this relation, $\mathbf{v}_e$ is the velocity of the emitted electron and $\mathbf{v}_{\text{mol}}$ is the mean speed of the molecule at 30 K. The largely different masses of the hydrogen isotopologues imply different values of $\mathbf{v}_{\text{mol}}$. Therefore, the broadening for T_2 is about $\Delta E = 148 \text{ meV}$, for HT is $\Delta E = 181 \text{ meV}$. Moreover, the different molecular masses imply a certain demixing effect along the beam axis.

- **Electron scattering with source molecules** The β -electrons which are guided to the spectrometer have a rather larger probability to undergo inelastic [2] and elastic scattering [36] with the molecules in the gas column. In these processes the energy and momentum of the electrons is changed. For example, the energy loss of the β -electrons by elastic scattering is given by [30]

$$\Delta E = 2 \frac{m_e}{m_{\text{mol}}} \cdot E \cdot (1 - \cos \theta) \quad (2.19)$$

which again depends on the molecular mass, m_{mol} . In general, the scattering angle θ is very small since the scattering is mostly forward peaked, which makes the contribution of the term in Eq. 2.19 quite low.

According to [37], the inelastic scattering cross-section is in first order proportional to the square of the intermolecular distance. This distance is related to the reduced mass of each isotopologue and thus the scattering cross-section will scale accordingly.

- **Final state distribution** In Eq. 2.5 the final energy states V_j were introduced to which a daughter molecule can be excited after the β -decay. The first electronic excited electronic state of $^3\text{HeT}^+$ appears at about 27 eV [55]. This rather large energy thus has no effect in the narrow region-of-interest around E_0 for the neutrino mass analysis at KATRIN. However, the nuclear recoil can give rise to a large number of rotational-vibrational states with a mean energy of about 1.89 eV for $^3\text{HeT}^+$ [12]. The energy states and the probabilities depend on the type of the daughter molecule, as shown in Fig. 2.7.

These systematic effects have been incorporated into the analysis models and simulation packages for KATRIN (e.g. see [25]). However, as input, they crucially require an accurate knowledge of the gas composition as provided by the laser Raman system.

In the KATRIN Design Report an estimate for the systematic uncertainty assigned to the description of the final state distribution is given. The shift on the neutrino mass square corresponding to this theoretical uncertainty is estimated to be $6 \times 10^{-3} \text{ eV}^2/c^4$ [30].

The isotopic composition weights the contributions of the final states from the different tritium containing isotopologues (T_2 , DT and HT). This means that systematic uncertainties in the measurement of the composition will additionally add up to the previously mentioned systematic shift. This additional impact resulting from the

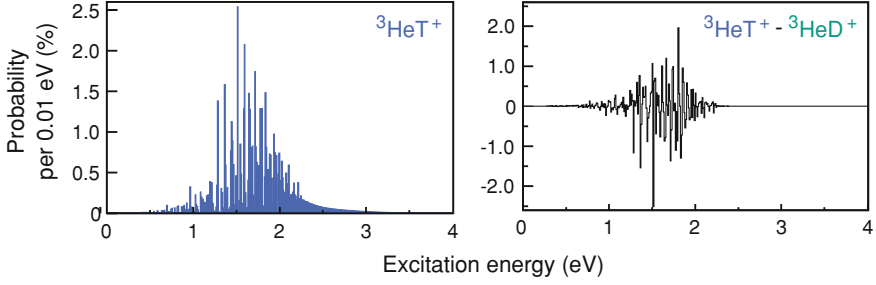


Fig. 2.7 Final state distributions. *Left panel* Final state distribution for the daughter molecule ${}^3\text{HeT}^+$. *Right panel* Difference of final state distributions of ${}^3\text{HeT}^+$ and ${}^3\text{HeD}^+$. It shows that the final state distributions are slightly different due to the different masses. Note that the nuclear recoil energy is already accounted for in these distributions

trueness of the LARA system was not considered by the Design Report. In general, a high trueness of an analytical system is achieved by an appropriate calibration. In Sect. 3.3, this topic is discussed in detail. In this context, calibration is understood as one or several methods to determine certain system-dependent factors which link the measured Raman signal to the actual composition. Thus, the calibration uncertainty of the Raman system is related to systematic errors in these factors.

At the beginning of the works related to this thesis, the uncertainty of $m(\nu_e)^2$ related to the calibration trueness was investigated. Dedicated simulations with the KATRIN simulation package, Kassiopeia [4], were performed, in close collaboration with Markus Hötzel and Wolfgang Käfer. These simulations contained a full WGTS model including all aforementioned species-dependent effects [25, 29]. The investigation strategy and the results were published soon after [57].

The dependence of the calibration uncertainty, $\sigma_{\text{cal,LARA}}$, and associated systematic shift, $\Delta m(\nu_e)^2$, is related to the tritium purity, ϵ_{T} . It is obvious, that the calibration of the system becomes irrelevant when the purity parameter approaches $\epsilon_{\text{T}} = 1$. Therefore, the investigations were performed by adopting the reference purity value of $\epsilon_{\text{T}} = 0.95$ (90 % T_2 , 10 % DT). In Fig. 2.8 the corresponding systematic shift of $m(\nu_e)^2$ is shown as a function of the LARA calibration error for an assumed vanishing neutrino mass ($m(\nu_e) = 0 \text{ eV}/c^2$). The relation between observed (measured) and true, relative tritium amount is given by

$$n_{\text{obs,T}_2,\text{rel}} = \frac{n_{\text{true,T}_2} \cdot (1 + \sigma_{\text{cal,LARA}})}{n_{\text{true,T}_2} \cdot (1 + \sigma_{\text{cal,LARA}}) + n_{\text{true,DT}}} \quad (2.20)$$

It can be deduced that the systematic shift in $\Delta m(\nu_e)^2$ would be $\leq 3 \times 10^{-3} \text{ eV}^2 \text{ c}^{-4}$ for realistic calibration errors $\sigma_{\text{cal,LARA}} \ll 50\%$.

In order to keep the combined systematic uncertainty from the description of the final-state distribution and the LARA calibration as low as possible, one aims for a calibration uncertainty of 10 % or smaller. In this case, the uncertainty contribution resulting from the trueness of the LARA calibration will not significantly contribute

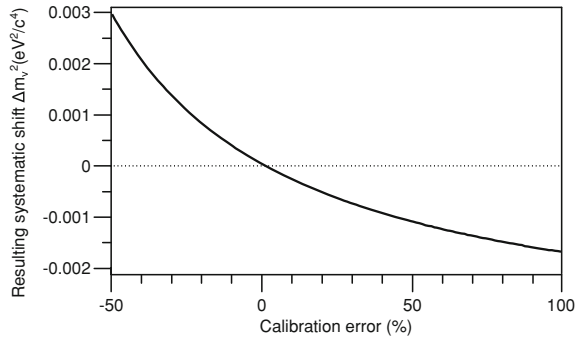


Fig. 2.8 Dependence of the systematic shift of $m(\nu_e)^2$ on the LARA calibration error. In this simplified case, the LARA calibration error ($\sigma_{\text{cal,LARA}}$) is defined as the percentage of misinterpretation of the calibration factor between the main species in the WGTS, T_2 and DT. The relation between observed (measured) and true, relative tritium amount is given by Eq. 2.20

to the total uncertainty [57]. Independent estimates using a toy model rather than the full source simulation lead to a comparable result [29].

Said considerations only account for the case of neutrino mass measurements by KATRIN in standard operation mode (i.e. isotopic purity $\epsilon_T \approx 0.95$ and measurements interval up to 30 eV below the endpoint energy). However, additional, auxiliary measurements are scheduled in which the knowledge of the gas composition is even more demanding. The energy loss function of the β -electrons inside the gaseous tritium source will be measured with the help of a mono-energetic electron-gun which probes the gas density and the characteristic energy loss of the scattered electrons [5]. Therefore, different source gas compositions will be prepared to disentangle the isotopic influence on the scattering losses. In this process the scenario changes from having only one primary constituent, T_2 , with the rest being only impurities, to a scenario with constituents of similar magnitude. Thus in the latter scenario, the same (relative) calibration uncertainties would imply larger (absolute) shift in the composition.

It is considered that KATRIN may also be utilized for the search of sterile neutrinos from the eV scale [19, 52] up to the keV scale [65], with the latter being a candidate for warm dark matter [1]. In these investigation the measurement interval will no longer be limited to the endpoint region of the spectrum, but be rather expanded to the entire spectrum. In this case much higher rates are present and significantly larger systematic effects with regard to gas dynamics and energy losses are expected. Thus, for these future investigations, the monitoring requirements are assumed to be even higher.

Summary of the accuracy issues of the KATRIN LARA system and objectives of this thesis An introduction to the Raman effect and its application for quantitative spectroscopy will be provided in Chap. 3. The feasibility of using Raman spectroscopy for the monitoring of the source gas composition was proved already in [35, 56, 59]. There, it could be demonstrated that the required precision of 0.1 % can

be achieved during a long-term test with circulating gas samples within a sampling time of 250 s [18, 60].

Following these early investigations, major optimizations in the experimental LARA setup, the data read-out and the data-processing methods were implemented in the course of this PhD thesis. These steps have enhanced the sensitivity of LARA by more than one order of magnitude as reported in Chap. 4 (experimental setup and routines).

Therefore, it can be claimed that the precision requirement of the KATRIN experiment is well-in-hand. On the other side, the fundamental open issue of calibration and thus of the LARA system's trueness was not touched prior to this thesis.

Therefore, the principle goal of this thesis was to develop different calibration strategies, to apply them and to further optimize them with regard to the LARA system of KATRIN, to validate them with regards to systematic uncertainty (trueness), and to finally evaluate the impact of the calibration to the neutrino mass analysis of KATRIN.

The path to this final goal is given along the chapters of this thesis. At the end of Chap. 3 various calibration possibilities will be discussed with regard to their individual advantages and drawbacks, from which the overall strategy for KATRIN will be identified. It consists of two approaches, which on their own would not be suitable for the calibration of the LARA system for all six hydrogen isotopologues. Only by combining these approaches the requirements can be met successfully. In Chap. 5, the first method is introduced which is able to cover all six hydrogen isotopologues. This approach is sample-free and is based on theoretical Raman intensities and the spectral sensitivity of the Raman system. However, the validity of the available theoretical data needs to be proved. This is done within a second, independent calibration method. Its methodology and results are discussed in Chap. 6. Finally, Chap. 7 is dedicated to the comparison of both calibration methods and to the discussion of their impact on the KATRIN physics analysis.

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