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Testing the Pauli Exclusion Principle with the VIP-2 Experiment

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Abstract: Violations of the Pauli Exclusion Principle (PEP), albeit small, could be motivated by physics beyond the Standard Model, ranging from violation of Lorentz invariance to extra space dimensions. This scenario can be experimentally constrained through dedicated, state-of-the-art X-ray spectroscopy, searching for a forbidden atomic transition from the L shell to the K shell already occupied by two electrons. The VIP-2 Experiment located at the underground Gran Sasso National Laboratories of INFN (Italy) tests PEP violations by introducing new electrons via a direct current in a copper conductor, measuring the X-ray energies through a silicon drift detector. Bayesian and frequentist analyses of approximately six months of data taken with the fully operational setup is presented, setting the strongest limit to date on the PEP violation shown by the VIP collaboration. The upper bound on PEP violation are placed at 90% CL $\beta^2/2 \leq 6.8 \times 10^{-42}$ with the Bayesian approach, and $\beta^2/2 \leq 7.1 \times 10^{-42}$ with the frequentist CL$_s$ technique.

Keywords: Pauli Exclusion Principle; X-rays; VIP-2; fundamental symmetries

1. Introduction

The Pauli Exclusion Principle (PEP) is a fundamental building block of modern physics, at the basis of many phenomena, from the stability of matter to neutron stars and from white dwarfs to superconductivity. In 1925, Wolfgang Pauli postulated that two electrons cannot occupy the same quantum state, in order to explain the electronic structure of the periodic table [1]. As quantum mechanics reached full development in the mid-1920s in the matrix formalism by Heisenberg, Born, and Jordan and in the wave function formalism by Schrödinger, PEP quickly became a fundamental pillar of the theory. The Symmetrization Postulate (SP) was formulated to assure either the symmetry or anti-symmetry of the states. PEP was subsequently generalized by Pauli and extended into the framework of relativistic quantum field theory, within the spin-statistics connection [2]. This theorem asserts that particles with half-integer spin, the fermions, are described by an antisymmetric wave function and follow the Fermi–Dirac statistics; particles with integer spin, the bosons, are described by a symmetric wave function and follow the Bose statistics. Yet, Pauli himself was unable to give a logical reason for the exclusion principle or to deduce it from more general assumptions [3]. Lüders and Zumino later demonstrated that the spin-statistics connection arises from a few general assumptions: Lorentz/Poincaré symmetry, CPT symmetry, and unitarity, locality, and causality [4]. Violations of the PEP can therefore be linked to fundamental concepts at the base of modern physics and the Standard Model itself. Extra space dimensions, violation of Lorentz invariance, non-commutative space-time, and discretized spacetime are often embedded in theories beyond the Standard Model and could therefore entail a PEP violation. Several experiments have been performed in the past searching for PEP violation, in the context of non-Paulian processes and charge non-conservation [5–7]. Depending on the theoretical framework, tiny violations could take place in *open* and *closed* systems. According to the Messiah–Greenberg (MG) [8] a superselection rule, transitions among states with different symmetries are forbidden. In this scenario, PEP could be tested only in open systems, namely those systems where the testing fermion is introduced from outside, making closed-system experiments searching for the stability of the matter insensitive to this search.

PEP violation was parametrized by Ignatiev and Kuzmin for electrons in terms of a three level Fermi oscillator, with β being the amplitude parameter connecting the forbidden states to allowed states [9]. Small violations are usually presented as a violation probability $\beta^2/2$. Greenberg and Mohapatra [10] suggested experimental methods, which led to the first experiment performed by Ramberg and Snow [11].

PEP was tested with electrons in copper atomic systems, introducing an electron from outside via a direct current. If a violation of PEP occurs, electrons introduced with the current form forbidden symmetry states with the electronic inner shell of the copper atoms. The process searched for in atomic systems is shown in Figure 1: on the left, a PEP-allowed transition $2p \to 1s$, where the $1s$ orbital is not full. On the right, a Pauli-forbidden transition where the $2p \to 1s$ happens even if the $1s$ orbital is already fully occupied.

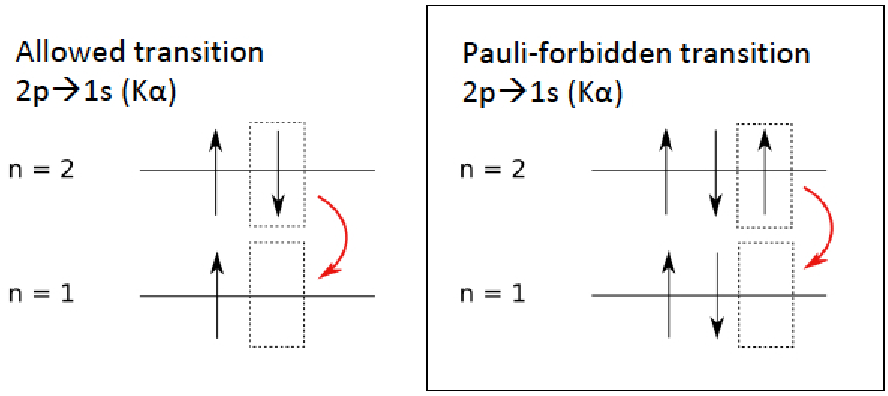

Figure 1. Overview of a standard K_α transition, **left**, and a PEP violating one, **right**. This process has a different X-ray emission energy, and can be searched for experimentally.

The energies of transitions that take place as the electron cascades down are influenced by the presence of the additional electron. As the $2p \to 1s$ transition occurs with the $1s$ orbital already occupied, the anomalous K_α transition caused by the PEP violating electrons would have a shift as a consequence of the additional shielding effect. This energy change is quantified in copper atoms to be around 300 eV for the K_α transitions [12,13]. Ramberg and Snow parametrized the $\beta^2/2$ probability in terms of the number of electron-atom interactions, assuming a motion of the injected electrons subjected to a scattering length μ. As no PEP forbidden emission line was detected in the X-ray spectrum, stringent limits were put on the violation probability, $\beta^2/2 < 1.7 \times 10^{-26}$. The VIP experiment was an improved version of the experiment carried out by Ramberg and Snow, located at the Gran Sasso underground laboratory and equipped with charge coupled devices for precision X-ray spectroscopy, and was able to improve the previous bound by more than two orders of magnitude [14].

The VIP-2 experiment is an upgrade of the VIP experiment, currently operating at the Gran Sasso national underground laboratory (LNGS). Its layout and improvements are listed in Section 2; the analysis strategy and the first results are presented in Section 3.

2. The VIP-2 Experiment

The VIP-2 experiment is located at the INFN's underground LNGS, in Italy. With an overburden of more than 3000 m water equivalent, the cosmic-ray background is greatly reduced. The cosmic muon flux rate is reduced by approximately six orders of magnitude. This low radioactivity environment is ideal to search for tiny effects such as the PEP violation. VIP-2 has the goal of reaching an exclusion of the PEP violation of $\beta^2/2 < 4 \times 10^{-31}$, two orders of magnitude better than the precedent VIP experiment. This is possible through the use of state-of-the-art radiation detectors, a bigger target, and a stronger direct current. Silicon drift detectors (SDDs) are ideal X-ray detectors, having an excellent spectroscopic response and a resolution of about 190 eV (FWHM) at 8 keV, and were developed in a collaboration between SMI, Politecnico di Milano, and the Fondazione Bruno Kessler [15]. Large geometrical acceptance and efficiency is a key requirement for X-ray detectors. With an overall active area of 0.64 cm^2, thickness of 450 µm, and efficiency of 99% at 8 keV, the SDD cell satisfy these requirements, allowing a sensible improvement with respect to charge coupled devices.

The section view of the VIP-2 experiment and the enclosing vacuum chamber are shown in Figure 2. The lateral view shows the copper target, realized as a pair of copper strips on both sides, each 71 mm long, 20 mm high, and 25 µm thick, where the direct current is circulated. With a peak current of 180 A, the copper strips are kept cool via a cooling pad in a closed chiller circuit. The pad is placed between the two strips. On each side of both copper strips, two SDD arrays are placed parallel to the target surface. Each array consists of a matrix of 2 × 4 SDD cells and is operated at a temperature of −90 °C. The vacuum chamber is kept at 10^{-5} mbar and contains the detectors and their front-end electronics. A Fe-55 radioactive source is present inside the chamber, used for the in-situ calibration of the SDDs, as explained below. Externally, a passive shield surrounds the vacuum chamber. An inner layer of copper bricks and an outer layer of lead bricks assure an enhanced suppression of environmental radiation, which is still present in the laboratory halls.

The VIP-2 experiment has been operating in its final configuration since 2019. Two different types of data taking, typically a month each, are alternated. With *current on*, the direct current is circulated in the copper target strips. Under the MG superselection rule, the new electrons test the PEP on each interaction with the copper atoms; if it is violated, anomalous X-rays emitted from the forbidden transitions would be detected. Data taking with current on therefore represents the signal. The *current off* data taking, instead, is used as reference and control in the data analysis.

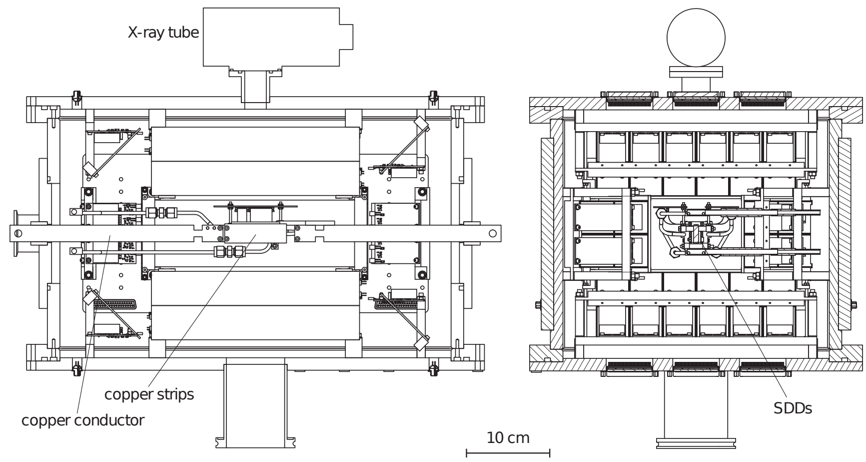

Figure 2. Lateral and frontal sections (on the left and on the right of the figure, respectively) of the VIP-2 apparatus. The copper strip target where the electrons are circulated is indicated on the left lateral section. The SDDs X-ray detectors are visible in the frontal section around the target. The apparatus is enclosed by the vacuum chamber.

Data

The data analyzed in this article correspond to approximately six months of experiment operation, from December 2019 to May 2020. The data were taken with a current of 180 A circulating in the target for approximately 83 days, and for 80 days without current circulating in the target. An in situ calibration is performed using fluorescence X-rays from manganese and titanium, the former from the Fe-55 decay and the latter from a 25 µm thick foil attached on top of the source. The calibration is executed in batches of approximately ten days, and for each SDD detector.

In Figure 3 the calibrated data acquired with and without current are shown, in blue and red, respectively. The PEP violation in copper is expected in the data with current, at a smaller energy with respect to the copper K_α line, around 7700 eV. The nickel present in the setup material is also visible with the K_α line at 7500 eV.

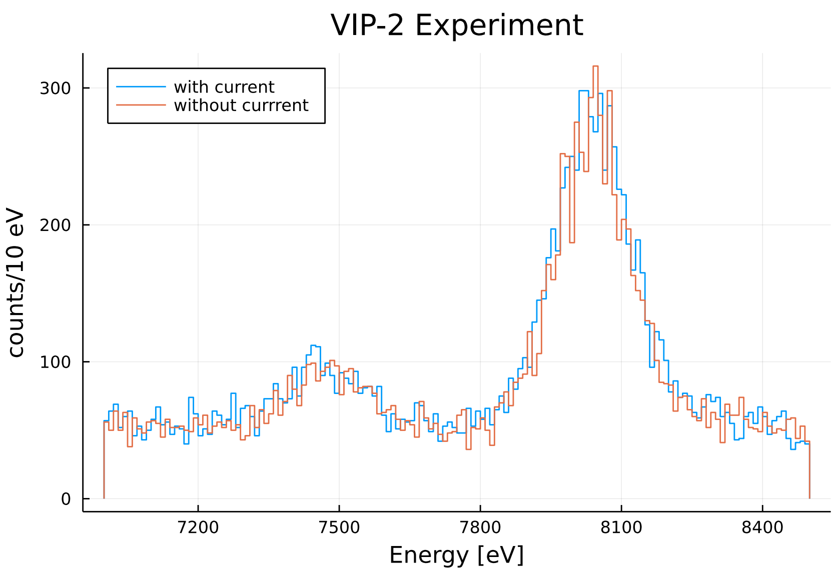

Figure 3. VIP-2 calibrated data in the region-of-interest 7000–8500 eV, corresponding to approximately six months of data taking between December 2019 and May 2020. The spectrum of the data acquired with a current of 180 A circulating in the target is shown in blue. The PEP violation signal is expected at around 7700 eV. Data acquired without current circulating in the target is used for reference and as control region in the data analysis and is shown in red. Both spectra show the copper and nickel K_α lines.

3. Data Analysis

The PEP violation in copper atoms would manifest itself with a forbidden transition, with respect to the standard one, due to the additional electromagnetic shielding provided by the already occupied 1s level. According to the MG superselection rule, this is expected only when fresh electrons are injected into the system by a direct current.

We performed both a Bayesian and a frequentist analysis using the data taken with current as signal spectrum, and the data taken without current as background control spectrum. The spectral shape description is the same in both. The continuum background is found to be optimally described by a first-degree polynomial. The copper and nickel lines are described by two Gaussian distributions each, accounting for the K_{α_1} and K_{α_2} components. Only in the signal spectrum another Gaussian distribution is used, for PEP-violating transitions centered at an energy of 7746 eV, and with the same resolution of the copper line.

3.1. Statistical Model

We call $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3, \theta_4, \theta_5)$ the vector of the parameters describing the spectral shape: center and resolution of the nickel line, center and resolution of the copper and PEP-violating line, and slope of the polynomial, respectively. Additionally, we call $\boldsymbol{y} = (y_1, y_2, y_3)$ the vector of the yields for the nickel (y_1), copper (y_2), and continuum background (y_3). The parameter of interest of the analysis, the signal yield, is denoted $\mathcal{S}$. The description of the spectra for the signal becomes:

$$\mathcal{F}^{wc}(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S}) = y_1 \times Ni(\theta_1, \theta_2) + y_2 \times Cu(\theta_3, \theta_4) + y_3 \times \mathrm{pol}_1(\theta_5) + \mathcal{S} \times PEPV(\theta_4). \quad (1)$$

For the control spectrum, it is instead:

$$\mathcal{F}^{woc}(\boldsymbol{\theta}, \boldsymbol{y}) = y_1 \times Ni(\theta_1, \theta_2) + y_2 \times Cu(\theta_3, \theta_4) + y_3 \times \mathrm{pol}_1(\theta_5) \quad (2)$$

where Ni and Cu described the K_α and K_β of nickel and copper, pol_1 is a first-order polynomial, and $PEPV$ is a Gaussian distribution used to represent the PEP violating line. The likelihood function can be written as:

$$\mathcal{L}(\mathcal{D}^{wc}, \mathcal{D}^{woc}|\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S}) = \mathrm{Poiss}(\mathcal{D}^{wc}|\mathcal{F}^{wc}(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S})) \times \mathrm{Poiss}(\mathcal{D}^{woc}|\mathcal{F}^{woc}(\boldsymbol{\theta}, \boldsymbol{y} \times \mathcal{R})) \quad (3)$$

where $\mathrm{Poiss}(n|x) = \frac{x^n}{n!}e^{-x}$, $\mathcal{D}^{wc}$ ($\mathcal{D}^{woc}$) is the spectrum in the signal (control) spectrum, and $\mathcal{R}$ is the ratio of the data acquisition times of the two spectra, which is used to normalize the yields of the background control spectrum. The parameters $\boldsymbol{\theta}$ and $\mathcal{R}$ are constrained through prior distributions in the Bayesian analysis and through penalty terms in the frequentist analysis. In particular, θ_1 and θ_3, the position of the nickel and copper lines, respectively, are constrained through a Gaussian within the experimental resolution of the energy scale; $\mathcal{R}$ is constrained also through a Gaussian to the ratio of the different data-taking time for $\mathcal{D}^{wc}$ and $\mathcal{D}^{woc}$. Finally, the parameter of interest, $\mathcal{S}$, has a flat prior, so it is left free in the frequentist analysis.

3.2. Bayesian Analysis

A Bayesian analysis using the outlined statistical model is performed on the VIP-2 experimental data, searching for PEP-violating events. The posterior probability can be expressed in terms of the likelihood function in Equation (3) and the priors $p(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S})$ via the Bayes and Laplace equation:

$$p(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S}|\mathcal{D}^{wc}, \mathcal{D}^{woc}) = \frac{\mathcal{L}(\mathcal{D}^{wc}, \mathcal{D}^{woc}|\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S})p(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S})}{\int d\boldsymbol{\theta} d\boldsymbol{y} \mathcal{L}(\mathcal{D}^{wc}, \mathcal{D}^{woc}|\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S})p(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S})}. \quad (4)$$

The inference about the parameter of interest $\mathcal{S}$ can be extracted via the marginalized probability:

$$p(\mathcal{S}|\mathcal{D}^{wc}, \mathcal{D}^{woc}) = \int p(\boldsymbol{\theta}, \boldsymbol{y}, \mathcal{S}|\mathcal{D}^{wc}, \mathcal{D}^{woc}) d\boldsymbol{\theta} d\boldsymbol{y} \quad (5)$$

from where the 90% posterior probability on the signal yield can be extracted. The numerical integration is performed using Markov-Chain Monte Carlo techniques via the BAT toolkit [16–18]. The posterior distribution for the parameter of interest is shown in Figure 4.

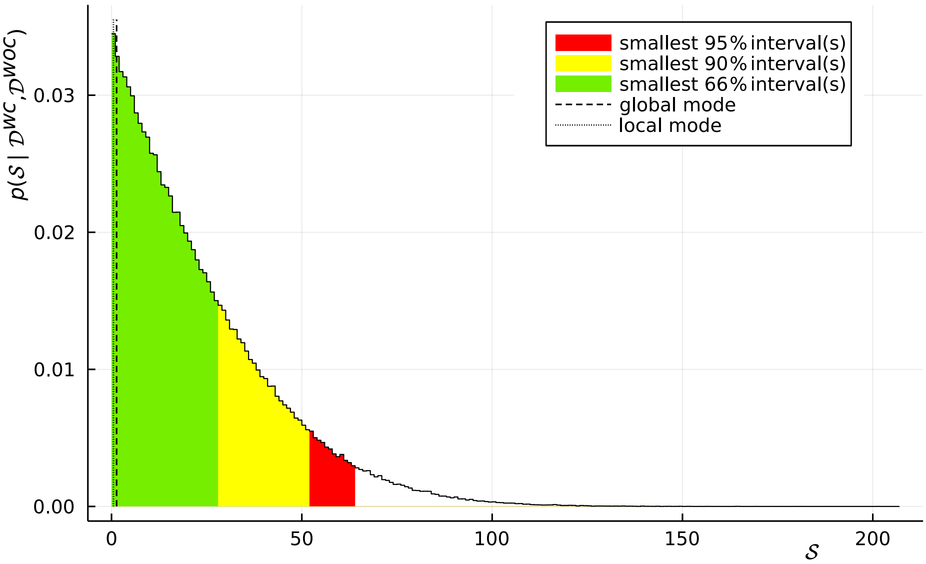

Figure 4. The posterior distribution for the signal yield $\mathcal{S}$ obtained by marginalization on all the parameters. Red, yellow, and green show the 95%, 90%, and 66% intervals, respectively.

The posterior shape for the data is exponentially falling, with the mode at $\mathcal{S} = 0$. From this probability density, 90% CL upper limit on the signal yield can be extracted, and is found to be:

$$\mathcal{S} \leq 52. \tag{6}$$

3.3. Frequentist Analysis

The (modified) frequentist CL_s analysis [19] of the VIP-2 experimental data also employs the same statistical description as in Section 3.1. A one-sided test statistic in the asymptotic approximation [20] based on the profile likelihood $\Lambda(\mathcal{S})$ is constructed as:

$$t_{\mathcal{S}} = -2\ln\Lambda(\mathcal{S}) = -2\ln\frac{\mathcal{L}(\hat{\hat{\boldsymbol{\theta}}}, \hat{\hat{\boldsymbol{y}}}, \mathcal{S})}{\mathcal{L}(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{y}}, \hat{\mathcal{S}})} \tag{7}$$

where $\mathcal{L}$ now incorporates multiplicative Gaussian penalty terms to represent the constraints arising from experimental uncertainties, interpreted as prior probabilities in the Bayesian description; $\hat{\hat{\boldsymbol{\theta}}}, \hat{\hat{\boldsymbol{y}}}$ in the numerator of Equation (7) are the parameters that maximize $\mathcal{L}$ for fixed $\mathcal{S}$, whereas $\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{y}}, \hat{\mathcal{S}}$ are the parameters that maximize the likelihood. The p-value is defined in terms of the probability distribution f under the parametrized signal hypothesis, and is written as:

$$p_{\mathcal{S}} = \int_{t_{obs}}^{\infty} f(t_{\mathcal{S}}|\mathcal{S})dt_{\mathcal{S}}. \tag{8}$$

The t_{obs} is the value of the test statistic for the observed VIP-2 data. The CL_s is a more robust way to represent exclusion limits. It is expressed in terms of the p-values for the signal $p_{\mathcal{S}}$ and background p_0 hypothesis:

$$\mathrm{CL}_s = \frac{p_{\mathcal{S}}}{1 - p_0} < 0.90. \tag{9}$$

The numerical computation is done with RooFit [21], used to obtain the observed and expected limits, which are shown in Figure 5 as a function of $\mathcal{S}$.

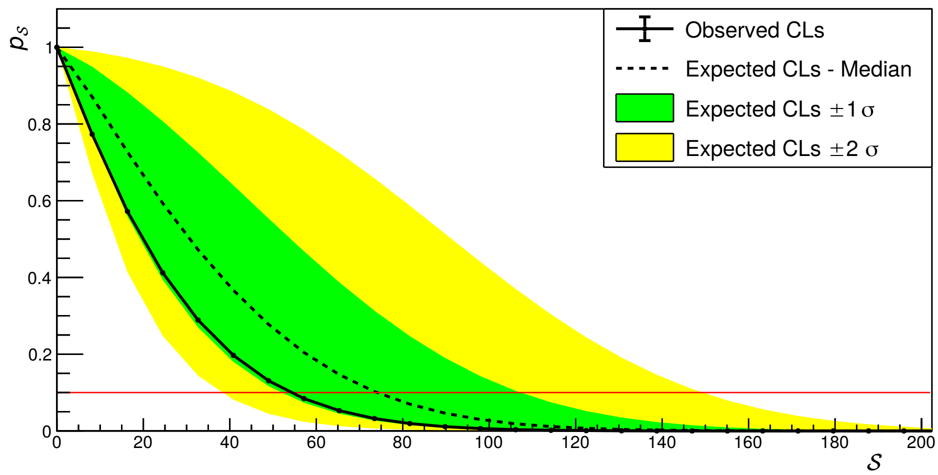

Figure 5. Observed (solid) and expected (dashed) CL_s limits as a function of the signal yield $\mathcal{S}$. The $\pm 1\sigma$ and $\pm 2\sigma$ around the expected limits are shown in green and yellow, respectively. The solid red line marks the 0.10 p-value.

The observed CL_s limit is stronger than the expected limit because of an under fluctuation of events in the region of the violating line; however, the two exclusion points are well withing one sigma. The 90% CL_s limit then results to be:

$$\mathcal{S} \leq 54. \tag{10}$$

3.4. Discussion

The 90% upper limit on the signal yield for the PEP violation with VIP-2 data considered in this article is $\mathcal{S} \leq 52$ with the Bayesian approach and $\mathcal{S} \leq 54$ using a frequentist CL_s. The upper limit on the number of signal events can be translated to an upper limit on the PEP violation probability, $\beta^2/2$, considering the data taking time with current, the current intensity, and the electron diffusion model [11,12,22]. Traditionally, since the experiment performed by Ramberg and Snow, the number of the electron-atom interactions in copper is expressed as $N_{int} = D/\mu$, with D the length of the copper target, and $\mu = 3.9 \times 10^{-6}$ cm the scattering length of electrons in copper. With this simple model, the upper limit on PEP violation is:

$$\beta^2/2 \leq 8.6 \times 10^{-31} \text{ (Bayesian)}, \qquad \beta^2/2 \leq 8.9 \times 10^{-31} \text{ (CL}_s\text{)}. \tag{11}$$

In recent years, a more realistic diffusion random walk model has been developed [22] already employed in open and closed systems [23,24], where the electron-atom interactions in copper occur with a characteristic time $\tau = 3.3 \times 10^{-17}$ s, also taking into account phonons and lattices irregularities. Within this model, the PEP is tested considerably more times with respect to the simple diffusion model. Under these assumptions, the upper limit on the PEP violation is:

$$\beta^2/2 \leq 6.8 \times 10^{-43} \text{ (Bayesian)}, \qquad \beta^2/2 \leq 7.1 \times 10^{-43} \text{ (CL}_s\text{)}. \tag{12}$$

4. Conclusions

The PEP is a cornerstone of quantum mechanics, sensible to theories beyond the Standard Model, which entail, e.g., extra space dimensions, violation of Lorentz invariance, non-commutative space-time, and discretized spacetime. Under the MG superselection rule, only electrons introduced from outside the system can violate the PEP; the VIP-2 experiment is able to test this scenario via a strong direct current that is circulated in a copper target. This article presents the analysis of the first set of data collected by the VIP-2 experiment at LNGS since the completion of the installation of the fully shielded setup. The data amount to approximately six months of data taking during December 2019–May 2020, with a current of 180 A circulating in the target for 83 days. The statistical analysis of the data was performed in a two-facet approach, Bayesian and frequentist. The 90% exclusion on $\beta^2/2$ is the stronger-than-ever limit put on the PEP violation of $\beta^2/2 \leq 6.8 \times 10^{-42}$ using a Bayesian approach and $\beta^2/2 \leq 7.1 \times 10^{-42}$ with the frequentist CL_s technique. The VIP-2 experiment continues the data-taking, aiming to further improve the limit set in this article. At the same time, the VIP-2 collaboration is investigating with theoreticians for the interpretation of the results and for future possible measurements.

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