

Leggett-Garg inequalities

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Abstract: A study on the Leggett-Garg inequalities, which determine if the classical hypothesis of macroscopic realism is true for observables at atomic and sub-atomic scale measured at different times. It is found that the bounds in the Leggett-Garg inequalities calculated under classical assumptions are violated when recalculating the Leggett-Garg inequalities under quantum mechanical assumptions. Finally, with the help of the results of an experiment based on neutrino flavour oscillations, it is found that classical assumptions are wrong.

I. INTRODUCTION

During the first half of the 20th century the foundations of quantum mechanics were established, the branch of physics which describe the phenomena that happen at atomic and sub-atomic scale. However, under this new theory a revolutionary idea appeared: The idea that instead of deterministic expressions, the phenomena and processes were described under probabilistic predictions. This idea, created quite the discussions between physicists who agreed to this description, like Niels Bohr, and physicists who thought that the probabilistic description was due that we lacked information and once we knew it, the phenomena would be described under deterministic expressions, like Albert Einstein.

As a matter of fact, Einstein, together with Boris Podolsky and Nathan Rosen wrote an article about the Einstein–Podolsky–Rosen paradox[1] the year 1935, where they described a thought experiment within the assumption of local realism (cause-and-effect are limited to the speed of light and the particle must have a pre-existing value for any measurement before any measurement is made). In this experiment, particles interacted in such a way that we could measure both their position and momentum more precisely than Heisenberg's uncertainty principle allows. Therefore, it proved that under local realism, quantum mechanics were incomplete and we needed a hidden variable theory. However, at 1964, John Stewart Bell wrote his article: On the Einstein Podolsky Rosen paradox[2], where he introduced the Bell inequalities, a series of inequalities which if local realism was true, they would be bounded by certain values, but when quantum correlations are considered, these bounds are broken and as such, this phenomena cannot be described under a local realism theory.

Inspired by Bell's inequalities, A. J. Leggett and Anupam Garg wrote at 1985 Quantum mechanics versus Macroscopic Realism: Is the Flux There when Nobody Looks?[3] where they introduced a series of inequalities based on measures in different times instead of measures of particles in a entangled state(a quantum state which cannot be factored as a product of states of its local constituents) moving back-to-back.

This introduction brings us to the ideas behind this TFG, the Leggett-Garg inequalities, which are used to see if macroscopic realism is true with the help of the correlations of measured observables at different times.

In this TFG we present the Leggett-Garg inequalities and their violation in a recent experiment performed with neutrinos, and finish with the conclusion.

II. THEORY

In order to begin, the theory section will start by describing the assumptions [3] under which classical predictions will be described: The first, the idea of macroscopic realism (A1), the idea that a macroscopic object, which has available two or more distinct states must be in a definite state at any given time. The second idea, that the system will be measured with a non invasive measure (A2), a measure which will not change the state of the system.

It will also be assumed that a measure on the observed system will return a macroscopic dichotomic variable $Q = \pm 1$, for which its two-time correlation function [4] $C_{ij} = \langle Q(t_i)Q(t_j) \rangle$ will be defined as:

$$C_{ij} = \sum_{Q_i, Q_j = \pm 1} Q_i Q_j P_{ij}(Q_i, Q_j) \quad (1)$$

where $Q(t_i) \equiv Q_i$ and $Q(t_j) \equiv Q_j$, P_{ij} is the probability of obtaining Q_i and Q_j .

Lastly, the n-form Leggett-Garg inequality will be defined as[4]:

$$K_n \equiv \sum_{i=1}^{n-1} C_{i+1,i} - C_{n,1} \quad (2)$$

Where this TFG will focus on the 3-form and 4-form: K_3 and K_4 .

Once the initial assumptions, variables and parameters are defined, the demonstration section starts by obtaining proof that under these classical assumptions, the 3-form of the Leggett-Garg parameter is bounded as:

$$K_3 \equiv C_{21} + C_{32} - C_{31} \leq 1 \quad (3)$$

A. Classical predictions

In order to prove (3), this TFG will obtain the bounds by two different approaches.

For the first one, the description of the probability of obtaining Q_i and Q_j will be in terms of a exhaustively defined system [4], a model where the hidden variables ζ and ζ' describe all the properties of the system exhaustively before and after the measure respectively.

The first step will be obtaining the expression for the probability of measuring Q_i and Q_j :

$$P(Q_i, Q_j) = \int d\zeta' d\zeta \xi_j(Q_j|\zeta') \gamma_i(\zeta'|Q_i, \zeta) \xi_i(Q_i|\zeta) \mu(\zeta) \quad (4)$$

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The measurement at t_{ij} is represented as function $\xi_{i/j}(Q_{i/j}|\xi)$, the function that describes how the measure will disturb the state of the system as $\gamma_i(\zeta'|Q_i, \zeta)$ and lastly, the probability distribution over the ζ and ζ' variables as $\mu(\zeta)$.

Because the condition (A2) is imposed, the measure will not disturb the state of the system, which gives the following condition: $\gamma_i(\zeta'|Q_i, \zeta) = \delta(\zeta' - \zeta)$:

$$P(Q_i, Q_j) = \int d\zeta \xi_j(Q_j|\zeta) \xi_i(Q_i|\zeta) \mu(\zeta) \quad (5)$$

By combining the two expressions used to define the correlation function (1):

$$\begin{aligned} \langle Q_i Q_j \rangle &= \int d\zeta \sum_{Q_i, Q_j = \pm 1} Q_i Q_j \xi_j(Q_j|\zeta) \xi_i(Q_i|\zeta) \mu(\zeta) \\ &= \int d\zeta \langle Q_i \rangle_\zeta \langle Q_j \rangle_\zeta \mu(\zeta) \end{aligned} \quad (6)$$

where $\langle \dots \rangle$ represents an expectation value of a variable ζ . Using this equation in (2) when $n=3$ and $n=4$:

$$K_3 = \int d\zeta [\langle Q_2 \rangle_\zeta \langle Q_1 \rangle_\zeta + \langle Q_3 \rangle_\zeta \langle Q_2 \rangle_\zeta - \langle Q_3 \rangle_\zeta \langle Q_1 \rangle_\zeta] \mu(\zeta) \quad (7)$$

$$\begin{aligned} K_4 = \int d\zeta [\langle Q_2 \rangle_\zeta \langle Q_1 \rangle_\zeta + \langle Q_3 \rangle_\zeta \langle Q_2 \rangle_\zeta \\ + \langle Q_4 \rangle_\zeta \langle Q_3 \rangle_\zeta \\ - \langle Q_4 \rangle_\zeta \langle Q_1 \rangle_\zeta] \mu(\zeta) \end{aligned} \quad (8)$$

Since the expectation value of $Q_i = \pm 1$, as defined under (A1), using table 1 is noted that for a measure for K_3 , it is obtained $K_3 = -3$ or 1 , therefore, for multiple measures, the average K_3 will be bounded as $-3 \leq K_3 \leq 1$. As observed, not only there is proof of expression (3), but there is also proof of a lower bound.

$\langle Q_1 \rangle_\zeta$	$\langle Q_2 \rangle_\zeta$	$\langle Q_3 \rangle_\zeta$	K_3
+	+	+	1
-	+	+	1
+	-	+	-3
+	+	-	1
-	-	+	1
-	+	-	-3
+	-	-	1
-	-	-	1

TABLE I: The value of K_3 for each possible combination of $\langle Q_i \rangle_\zeta$, where +1 is written as + and -1 as -.

Similarly for K_4 using table 2, the bounds for an average K_4 are described as $-2 \leq K_4 \leq 2$.

$\langle Q_1 \rangle_\zeta$	$\langle Q_2 \rangle_\zeta$	$\langle Q_3 \rangle_\zeta$	$\langle Q_4 \rangle_\zeta$	K_4
+	+	+	+	2
-	+	+	+	2
+	-	+	+	-2
+	+	-	+	-2
+	+	+	-	2

-	-	+	+	-2
-	+	-	+	2
-	+	+	-	-2
+	-	-	+	-2
+	-	+	-	2
+	+	-	-	-2
-	-	-	+	2
-	-	+	-	-2
-	+	-	-	-2
-	-	-	-	2
-	-	-	-	2

TABLE II: The value of K_4 for each possible combination of $\langle Q_i \rangle_\zeta$, where +1 is written as + and -1 as -.

The second approach will be proven by using the correlation function C_{ij} obtained from the joint probability $P_{ij}(Q_i, Q_j|1)$ and simply obtaining all possible combinations.

Under assumption (A1), observable Q always has a well-defined value, so the two-time probability can be obtained from [4]:

$$P_{ij}(Q_i, Q_j) = \sum_{Q_k, k \neq i, j} P_{ij}(Q_3, Q_2, Q_1) \quad (9)$$

$$\begin{aligned} (e.g. P_{12}(Q_1, Q_2) = P_{12}(+, Q_2, Q_1) \\ + P_{12}(-, Q_2, Q_1)) \end{aligned}$$

However, due to assumption (A2), the state of the system will not be affected by the measure, therefore, the order at which the measure is realized is irrelevant, and $P_{ij}(Q_3, Q_2, Q_1) = P(Q_3, Q_2, Q_1)$.

The correlation functions for K_3 are as follows, where +1 is written as + and -1 as -:

$$\begin{aligned} C_{21} = P(+, +, +) - P(+, +, -) - \\ P(-, -, +) + P(-, -, -) - P(+, -, +) + \\ P(+, -, -) + P(-, +, +) - P(-, +, -) \end{aligned} \quad (10)$$

$$\begin{aligned} C_{32} = P(+, +, +) + P(+, +, -) + \\ P(-, -, +) + P(-, -, -) - P(+, -, +) - \\ P(+, -, -) - P(-, +, +) - P(-, +, -) \end{aligned} \quad (11)$$

$$\begin{aligned} C_{31} = P(+, +, +) - P(+, +, -) - \\ P(-, -, +) + P(-, -, -) + P(+, -, +) - \\ P(+, -, -) - P(-, +, +) + P(-, +, -) \end{aligned} \quad (12)$$

After all the C_{ij} are obtained, they will be used in expression (2) with $n=3$, and thanks to $\sum_{Q_1, Q_2, Q_3} P(Q_3, Q_2, Q_1) \equiv 1$, the following expression is obtained:

$$K_3 = 1 - 4[P(+, -, +) + P(-, +, -)] \quad (13)$$

The choice of $P(+, -, +) = P(-, +, -) = 0$ yields the upper bound 1, and $P(+, -, +) + P(-, +, -) = 1$ yields the lower bound -3, the same bounds found with the other approach, further solidifying our proof.

For K_4 using the previous method:

$$\begin{aligned}
K_4 = & 2 - 4[P(+, -, +, +) + \\
& P(-, +, +, -) + P(-, -, +, -) + \\
& P(+, +, -, +) + P(+, -, -, +) + \\
& P(-, +, -, -) + P(+, -, +, -) + \\
& P(-, +, -, +)] \quad (14)
\end{aligned}$$

which with analogous procedure as before, yields $-2 \leq K_4 \leq 2$,

Once is proven that K_3 and K_4 are bounded, the question of how a K_n would be classically bounded is answered by[4]:

$$\begin{aligned}
-n \leq K_n \leq n - 2 \text{ if } n \text{ odd} \\
-(n - 2) \leq K_n \leq n - 2 \text{ if } n \text{ even} \quad (15)
\end{aligned}$$

The reasoning behind this bounds being as follows: Thanks to expression (6), it is known that $\langle Q_i \rangle \cdot \langle Q_j \rangle$ can be used to replace $\langle Q_i \cdot Q_j \rangle$, so building any K_n using (2) and the definition of C_{ij} , an absolute maximum value of $n-1$ is obtained for $\sum_{i=1}^{n-1} C_{i+1,i}$.

In order to obtain the upper bound, $\sum_{i=1}^{n-1} C_{i+1,i}$ needs to be maximized, achieved by imposing that all the $\langle Q_i \rangle$ must be equal, doing this procedure, $\sum_{i=1}^{n-1} C_{i+1,i}$ is equal to $n-1$, however, as there is a $-\langle Q_n \rangle \cdot \langle Q_1 \rangle$, it makes the upper bound $n-2$.

For the lower bound, due to its construction, the sum of $\langle Q_{i+1} \rangle \cdot \langle Q_i \rangle$ has to be negative. Therefore, the following condition is obtained, $\langle Q_{i+1} \rangle = -\langle Q_i \rangle$.

It is also observed that all the terms can be expressed as $\langle Q_{i \text{ odd}} \rangle \cdot \langle Q_{i \text{ even}} \rangle$, from which is extracted the condition that in order to obtain the lowest possible value, $-(n+1)$, $\langle Q_{i \text{ even}} \rangle = -\langle Q_{i \text{ odd}} \rangle$.

But, K_n is not only the sum term, there's also a $\langle Q_n \rangle \cdot \langle Q_1 \rangle$, which under the previous condition, is $+1$ if n is even or -1 if n is odd, which makes the lower bound for K_n $-n$ if n is odd and $-n+2$ if n is even.

B. Quantum mechanical predictions

Once the classical bounds are obtained and proven, the task will change to redoing the same procedures but under quantum mechanics in order to see if differences appear in the bounds we obtain[5].

First, operator Q returns the value $+1$ when $|+1\rangle$ is measured and the value -1 when $|-1\rangle$ is measured, therefore, the projection of operator Q will be $\frac{1+a}{2}$, where a is the value obtained in the measure.

Second, the expression of the joint probability (used to define expression (1)) of obtaining for Q_i outcome $a = \pm 1$ and for Q_j outcome $b = \pm 1$ is:

$$\begin{aligned}
P(a, b) = & \langle \psi | \frac{1+aQ_i}{2} \cdot \frac{1+bQ_j}{2} \cdot \frac{1+aQ_i}{2} | \psi \rangle = \frac{1}{4} + \\
& \frac{1}{4} a \langle \psi | Q_i | \psi \rangle + \frac{1}{8} b \langle \psi | Q_j | \psi \rangle + \\
& \frac{1}{8} ab \langle \psi | \{Q_i, Q_j\} | \psi \rangle + \frac{1}{8} b \langle \psi | Q_i Q_j Q_i | \psi \rangle \quad (16)
\end{aligned}$$

With the use of (1), $C_{ij} = \sum_{a,b=\pm 1} abP(a, b)$, and using the previous notation, C_{ij} can be expressed as:

$$C_{ij} = \frac{1}{2} \langle \psi | \{Q_i, Q_j\} | \psi \rangle \quad (17)$$

However, it is also possible to work with vectors, in such case, Q_i is equal to $\vec{a}_i \cdot \vec{\sigma}$, where \vec{a}_i is a unit vector for t_i and $\vec{\sigma}$ is a vector of Pauli matrices.

Expressing (17) in this new definition, the products of $(\vec{a}_i \cdot \vec{\sigma}) \cdot (\vec{a}_j \cdot \vec{\sigma})$ obtained in the anticommutation due to the redefinition of Q_i are equal to $(\vec{a}_i \cdot \vec{a}_j)I + i(\vec{a}_i \times \vec{a}_j) \cdot \vec{\sigma}$, and remembering that the anticommutation of two Pauli matrices are zero, the alternative expression is obtained:

$$C_{ij} = \vec{a}_i \cdot \vec{a}_j \quad (18)$$

Once the correlation function for quantum mechanics is obtained, using expression (18) the rebuilt $K_n(2)$ in terms of unit vectors for each t_i is:[4]

$$K_n = \sum_{i=1}^{n-1} \vec{a}_{i+1} \cdot \vec{a}_i - \vec{a}_n \cdot \vec{a}_1 \quad (19)$$

Where defining θ_i as the angle between vectors \vec{a}_{i+1} and \vec{a}_i , equation (19) turns into:

$$K_n = \sum_{i=1}^{n-1} \cos \theta_i - \cos \left(\sum_{i=1}^{n-1} \theta_i \right) \quad (20)$$

And if K_3 and K_4 are represented, the maximum values obtained are $3/2$ and $2\sqrt{2}$ respectively.

It is observed that they violate the bounds of K_3 and K_4 described under classical predictions (1 and 2 respectively). This is an important result, because thanks to this difference of boundaries, it is possible to check with the construction of K_3 or K_4 if the system behaves classically or quantum mechanically by the range of values obtained during the measure.

An example of how the theory would be applied would be supposing that the system evolves under the following toy model Hamiltonian:

$$H = \frac{\Omega \sigma_x}{2}$$

As such, the time evolution operator will assume the form:

$$\begin{aligned}
U = & \cos(\Omega(t_j - t_i) \cdot 1/2)I - \\
& i \sin(\Omega(t_j - t_i) \cdot 1/2)\sigma_x \quad (21)
\end{aligned}$$

Defining operator $Q(t_i) \equiv Q_i$ as $Q_i = \sigma_z$, Q_j will be obtained applying the time evolution operator to Q_i :

$$\begin{aligned}
Q(t_j) \equiv Q_j \equiv U^\dagger(t_j - t_i) \cdot Q_i \cdot U(t_j - t_i) = \\
\cos(\Omega(t_j - t_i))\sigma_z \quad (22)
\end{aligned}$$

And for simplicity, it is assumed that the time intervals between measures are equal, $t_{i+1} - t_i = \tau$.

For obtaining C_{ij} expression (17) will be used and for K_n it is obtained:

$$\begin{aligned}
K_n = & (n - 1) \cos(\Omega\tau) \\
& - \cos((n - 1)\Omega\tau) \quad (23)
\end{aligned}$$

This expression, which if $n=3$ is represented as:

$$K_3 = 2 \cos(\Omega\tau) - \cos(2\Omega\tau) \quad (24)$$

and the graphical representation is as follows:

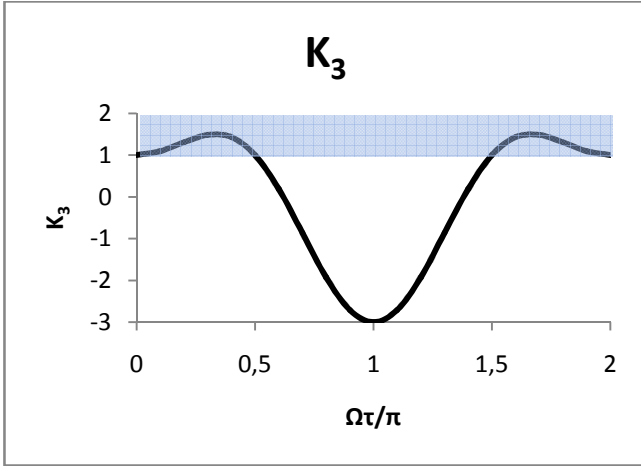


FIG. 1: The graphical representation of K_3 in (24) for $\Omega\tau$, where the region where the values are forbidden under classical predictions is shaded.

And for $n=4$, the expression and representation are as follows:

$$K_4 = 3 \cos(\Omega\tau) - \cos(3\Omega\tau) \quad (25)$$

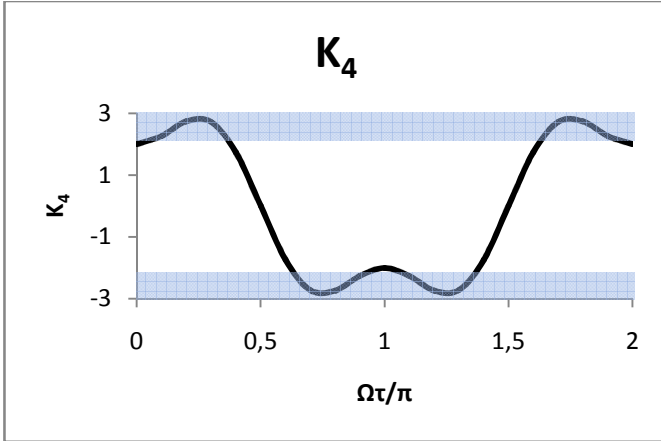


FIG. 2: The graphical representation of K_4 in (25) for $\Omega\tau$, where the region where the values are forbidden under classical predictions is shaded.

As it is seen, under quantum mechanical evolution, the Leggett-Garg inequalities are violated, as explained before. It is also observed that for K_3 , only the upper bound is relevant, but for K_4 both bounds are important.

III. EXPERIMENT

Once the theory is explained, the following step will be to prove if the Leggett-Garg inequalities are violated or not in reality with the help of realized experiments, where a comparison will be realized between the theory predictions and the data obtained.

In this TFG the experiment used is based on the violation of the Leggett-Garg inequalities in neutrino flavour oscillations[6].

This experiment studies the oscillation of neutrino flavours between the muon and the electron neutrinos. As such, it is assigned the observable Q to neutrino flavours as $Q|v_\mu\rangle = |v_\mu\rangle$ and $Q|v_e\rangle = -|v_e\rangle$, for muon- and electron-neutrino states respectively.

In order to compare the theory with the data obtained, the prediction will be calculated by the predicted time evolution of Q for a time interval t_j-t_i under the following Hamiltonian for neutrino propagation given by (with $\hbar=c=1$)[6]:

$$\begin{aligned} H &= \left(p + \frac{m_{\nu e}^2 + m_{\nu \mu}^2}{4p} + \frac{V_C}{2} + V_N \right) I \\ &+ \frac{1}{2} \begin{pmatrix} V_C - \omega \cos 2\theta & \omega \sin 2\theta \\ \omega \sin 2\theta & \omega \cos 2\theta - V_C \end{pmatrix} \\ &\equiv r_0 I + \frac{\vec{r} \cdot \vec{\sigma}}{2} \end{aligned} \quad (26)$$

Where a time evolution operator U will be calculated.

θ is the neutrino vacuum mixing angle, measured as 38.54° [7], $m_{\nu \mu}$ and $m_{\nu e}$ are the mass of the respective neutrinos, $\omega \equiv (m_{\nu \mu}^2 - m_{\nu e}^2)/2p$ is the oscillation

frequency, experimental data gives the value of $(m_{\nu \mu}^2 - m_{\nu e}^2) = 2.41 \times 10^{-3} \text{ eV}^2$ [7]. $V_{C/N} = \sqrt{2} G_F n_{e/n}$ is the charged/neutral current potential due to coherent forward scattering of neutrinos with electrons/neutrons in matter and G_F is the Fermi coupling constant, however, since it is considered that matter effects are negligible in this case, $V_{C/N} \approx 0$.

Since the term proportional to the identity matrix I affects all flavour states identically it will not contribute to flavour oscillations, also since this experiment is in the relativistic limit, it is possible to approximate p for E as the relativistic neutrino momentum-energy.

Considering $H_{\text{osc}} \equiv \frac{\vec{r} \cdot \vec{\sigma}}{2}$, with $\vec{r} = (r_x, 0, r_z) = (\omega \sin 2\theta, 0, -\omega \cos 2\theta)$, it is obtained the time evolution operator U as:

$$U(\omega: t_i, t_j) \equiv U(\psi_{ij}) = \cos(\psi_{ij}) I - i \sin(\psi_{ij}) (r_x \cdot \sigma_x + r_z \cdot \sigma_z) \quad (27)$$

Where the oscillation frequency ω for energy E is expressed in the phase ψ_{ij} as:

$$\psi_{ij} \approx \frac{\omega}{2} (t_j - t_i) \quad (28)$$

If \hat{Q}_i is defined as $\hat{Q}_i \equiv \sigma_z$, and with the help of the time evolution operators, \hat{Q}_j is obtained as:

$$\begin{aligned} \hat{Q}_j &= U(\psi_{ij})^\dagger \hat{Q}_i U(\psi_{ij}) \\ &= \cos(\psi_{ij})^2 \sigma_z \\ &+ \sin(\psi_{ij})^2 (1 - 2r_x^2) \sigma_z \\ &+ 2 \sin(\psi_{ij})^2 r_x r_z \sigma_x \\ &+ 2 \sin(\psi_{ij}) \cos(\psi_{ij}) r_x \sigma_y \end{aligned} \quad (29)$$

By using the correlation function (17):

$$C_{ij} = 1 - 2 \sin(\psi_{ij})^2 \sin(2\theta)^2 \quad (30)$$

And using this result, and considering that $t_{i+1} - t_i = \tau$, the theoretical K_4 is:

$$\begin{aligned}
K_4 &= 2 + 2 \sin(3\psi_{ij})^2 \sin(2\theta)^2 \\
&\quad - 6 \sin(\psi_{ij})^2 \sin(2\theta)^2
\end{aligned} \quad (31)$$

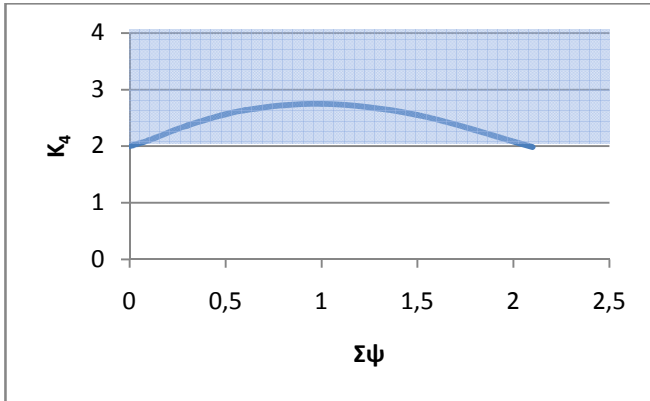


FIG. 3: The graphical representation of the theoretical K_4 (31) versus the sum of relative phase (used instead of the relative phase in order to better compare the theoretical prediction with the data) considering $\sin(2\theta)^2 = 0.95$ [7], where the region where the values are forbidden under classical predictions is shaded.

The data was gathered by the MINOS neutrino experiment[7], which measures a beam initially consisting of 98% muon-neutrinos with an energy range of 0.5-50 GeV.

Taking a look at the experiments results:

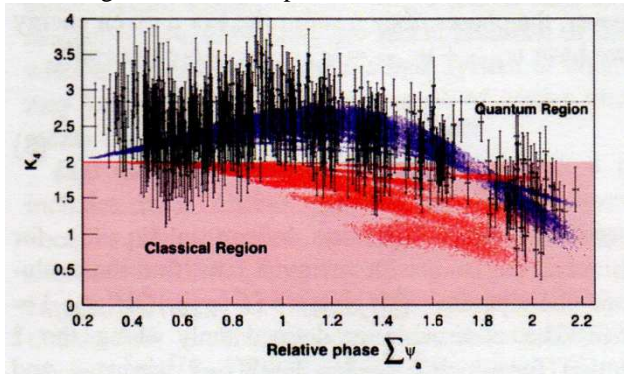


FIG. 4: The distribution of K_4 versus the sum of the phases ψ_{ij} obtained from the experiment.

Figure obtained from [6] J.A. Formaggio, D. I. Kaiser, M.M. Murskyj and T.E. Weiss, Violation of the Leggett-Garg Inequality in Neutrino Oscillations, PRL 117, 050402 (2016)

It is observed that not only the values obtained are a clear violation of the Leggett-Garg inequalities (and as such proof that macroscopic realism is not true for neutrinos) but that the values follow the quantum mechanical prediction, which suggests that quantum mechanics are the correct method to describe atomic and sub-atomic phenomena.

IV. CONCLUSIONS

- As seen with the theory, under the hypothesis of macroscopic realism and that a non-invasive measure is realized, the bounds obtained on the construction of K_n (the Leggett-Garg parameter, defined as a series of correlation functions in (2)) under classical predictions are broken when K_n is constructed under quantum mechanical predictions. Therefore, by comparing the range of values obtained during a measure, it is possible to check if classical predictions in this scale are correct or not.
- Thanks to the experiment, there is data to check if macroscopic realism is true in atomic and sub-atomic scale. As seen, data suggests a violation of the Leggett-Garg inequalities and proof that suggests that the phenomena in this scale behaves as quantum mechanics predicts.

Acknowledgments

I would like to thank my advisor for his help, the director, my friends and family for their support and finally the reader, for his or her attention.

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