Leggett-Garg tests for macrorealism: interference experiments and the simple harmonic oscillator.

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Abstract

Leggett-Garg (LG) tests for macrorealism were originally designed to explore quantum coherence on the macroscopic scale. Interference experiments and systems modelled by harmonic oscillators provide useful examples of situations in which macroscopicity has been approached experimentally and may be turned into LG tests with a dichotomic variable $Q$ by simple partitionings of a continuous variable such as position. Applying this approach to the double-slit experiment in which a measurement at the slits and screen are considered, we find that LG violations are always accompanied by destructive interference. The converse is not true in general and we find that there are non-trivial regimes in which there is destructive interference but the two-time LG inequalities are satisfied which implies that it is in fact often possible to assign (indirectly determined) probabilities for the interferometer paths. Similar features have been observed in recent work involving a LG analysis of a Mach-Zehnder interferometer and we compare with those results. We also compare with the related problem in which a more direct determination of the paths is carried out using a variable-strength measurement at the slits and the resulting deterioration of the interference pattern is examined. We extend the analysis to the triple-slit experiment. We find examples of some surprising relationships between LG inequalities and NSIT conditions that do not exist for dichotomic variables, including a violation of the Lüders bound. We analyse a two-time LG inequality for the simple harmonic oscillator. We find an analytically tractable example showing a two-time LG violation with a gaussian initial state, echoing recent results of Bose et al (Phys. Rev. Lett. 120, 210402 (2018)).

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I. INTRODUCTION

The Leggett-Garg (LG) inequalities were proposed in order to test the world view known as macrorealism, the view that a macroscopic object evolving in time may possess definite properties independent of past or future measurements [1] [2]. The main motive for developing such tests is that they offer the possibility of assessing whether macroscopic objects may exist in coherent superpositions. An affirmative answer to this question would rule out interesting families of alternatives to quantum theory in which macroscopic superpositions are suppressed [3].

LG tests typically concern measurements of a single dichotomic variable $Q$ in experiments involving either single times or pairs of times thereby determining the averages $\langle Q_i \rangle$ and correlators $C_{ij} = \langle Q_i Q_j \rangle$, where $Q_i$ denotes $Q(t_i)$ and $i, j = 1, 2, 3$. Macrorealism is characterized by three requirements: (i) macrorealism per se (the variables take definite values); (ii) non-invasive measurability (the present state cannot be affected by a past measurement), (iii) induction (future measurements cannot affect the present state). These assumptions ensure the existence of a joint probability distribution at three times on the variables $Q_i$ which in turn implies that the averages and correlators obey the following two types of inequality: the three-time LG inequalities,

\[ 1 + C_{12} + C_{23} + C_{13} \geq 0, \]  
(1.1)

plus the three more obtained by flipping the sign of each $Q_i$, and the two-time LG inequalities,

\[ 1 + \langle Q_i \rangle + \langle Q_j \rangle + C_{ij} \geq 0, \]  
(1.2)

plus three more from the same sign flips, where $ij = 12, 23, 13$. For a three-time situation there are a total of four three-time LG inequalities and twelve two-time inequalities. This set of sixteen form a set of conditions for macrorealism which are both necessary and sufficient [4]. However, purely for experimental convenience it is often simpler to work solely with the two-time LG inequalities and indeed many of the experiments testing the LG inequalities do precisely this. Necessary and sufficient conditions of this general form have also been found for multi-time measurements [5] and many-valued variables [6].

Although there has been considerable theoretical development of the LG framework over the years and numerous experimental tests (see Ref.[7] for a useful review), these tests usually
involve very simple spin systems and it would probably be fair to say that a truly macroscopic experimental test has yet to be performed. In the light of this, one way to proceed would be to examine different types of experiments which were not originally designed to be LG tests but were designed to explore macroscopicity. Happily, there are at least two classes of systems which fit the bill. First, as noted by Pan [8], interference experiments have now been developed to the point that interference effects can be detected for sizeable objects, with reasonable claim of macroscopicity [9]. Second, a number of recent experiments have shown it is possible to trap reasonably large masses in harmonic wells [10]. Hence it is clearly of considerable interest to develop LG tests for both interference experiments and simple harmonic oscillators and this is what we do in this paper.

We first analyze the traditional double slit experiment from the perspective of the LG framework, modestly generalized (along the lines discussed in Ref.[6]) to take into account the specific features of the experiment. We first outline in Section 2 the theoretical background and experimental procedure whereby a double-slit experiment is turned into a LG test. We then examine, in Section 3, the relationship between the Leggett-Garg inequalities for the particle paths and the interference pattern, thereby establishing what connection exists between two quite different notions of quantumness. We find that LG violations are always accompanied by destructive interference, hence these two different notions of quantumness are related. But the converse is not true and we find significant regimes in which there is destructive interference but the LG inequalities are satisfied. This sheds some light on the old question as to the degree to which one can assign probabilities to the particle paths in an interference experiment when destructive interference is present – it is in fact possible for a set of indirectly constructed probabilities. Our work has some overlap with a recent proposal by Pan to use a Mach-Zehnder interferometer for a LG test, and we discuss connections with his work [8].

We then explore in Section 4 a different but related question in this situation, which is the question as to whether one can actually measure which slit the particle went through without disturbing the interference pattern. This has been investigated previously, but here we make use of the formalism we developed to give a brief answer to this question, using a variable strength measurement at the slits to give an approximate determination. We find a link to the LG approach in the limit of a weak measurement.

In Section 5 we extend our considerations to the triple-slit experiment which has some
interesting new features. The relationship between destructive interference and LG violation is more fluid. However what is of perhaps greater interest is that the triple-slit experiment provides an arena in which some of the macrorealism conditions for many-valued variables proposed in Ref.\[6\] can be put to experimental test. In particular, this system shows a non-trivial relationship between LG violations and no-signaling in time (NSIT) conditions (unlike systems with dichotomic variables for which the latter simply implies the former). We also find possible violations of the Lüders bound (the maximal LG violation allowable by quantum mechanics for measurements of dichotomic variables, numerically the same as the Tsirelson bound \[11\] in Bell experiments).

In Section 6, we investigate a set of two-time LG inequalities for the simple harmonic oscillator whose initial state is a coherent state, inspired by the general programme initiated by Bose et al \[10\]. We find exact analytic expressions for the averages and single correlator and exhibit a regime in which LG violation is possible. We identify the origin of the LG violation in this case and contrast with that arising in interference experiments. This part of our work is also a natural progression from a recent work in which a LG analysis of the free particle and the arrival time problem was carried out \[12\].

We summarize and conclude in Section 7.

II. GENERAL ANALYSIS OF MEASUREMENTS AT TWO TIMES FOR THE DOUBLE SLIT EXPERIMENT

Although the LG framework is usually framed in purely macrorealistic terms, it turns out to be most convenient here to begin with a brief quantum-mechanical description of the double slit experiment. We consider motion in the $xy$ plane with the slits and screen taken to be lines of constant $y$ and consider an incoming state $\rho$ approaching the slits in the $y$ direction. See Figure 1.

At $t_1$ there is a projective measurement described by projection operator $P_s$ onto values $s = \pm 1$ denoting which slit the particle went through (which could simply be projections on to the positive or negative $x$-axis) and followed by time evolution to time $t_2$ and second projective measurement $E_n$ onto one of many values $n$, denoting a coarse-grained measurement
FIG. 1: The experimental setup for the double-slit. The slits are centered at \( x = \pm L \) and \( y = 0 \). The particle propagates from the slit to the screen at \( y = D \) where the interference pattern is measured.

of the screen position. We write this projector

\[
E_n = \int_{\Delta_n} dx \ |x \rangle \langle x|.
\]  

(2.1)

Here, \( \Delta_n \) denotes one of many small intervals which divide up the real line, each of size \( \Delta \). Generally each \( \Delta_n \) is taken to be arbitrarily small but may be kept for normalization purposes. (Following Ref. [6], we use \( P_s \) for projections onto dichotomic variables and \( E_n \) for projections onto variables with three or more values).

The two-time probability for these sequential measurements is,

\[
p_{12}(s_1, n_2) = \text{Tr} \left( E_n(t_2) P_{s_1}(t_1) \rho P_{s_1}(t_1) \right).
\]  

(2.2)

(The formalism given here follows Ref. [13]). It matches the single time probability \( p_1(s_1) = \text{Tr}(P_{s_1}(t_1) \rho) \) when summed over \( n_2 \). The interference pattern at the screen is given by the probability

\[
p_2(n_2) = \text{Tr}(E_n(t_2) \rho),
\]  

(2.3)

in which there is no earlier measurement at \( t_1 \). (Here the subscripts on the probabilities denote the quantities measured). It does not coincide with Eq. (2.2) summed over \( s_1 \), i.e.
the so-called no-signaling in time (NSIT) condition \[14, 15\]

\[
p_2(n_2) = \sum_{s_1} p_{12}(s_1, n_2), \tag{2.4}
\]
is not satisfied in general. This is the familiar fact that sequentially measured probabilities for pairs of paths in the double slit experiment suffer from interference and fail to satisfy the probability sum rules.

Here, however, we are concerned with looking for other, indirect procedures for determining possible probabilities for the paths in a double slit experiment. In particular, we consider the quasi-probability,

\[
q(s_1, n_2) = \text{ReTr} \left( E_{n_2}(t_2) P_{s_1}(t_1) \rho \right). \tag{2.5}
\]

(See Refs.\[13, 16, 17\]). This quantity does match the two marginals, \(p_1(s_1)\) and \(p_2(n_2)\), and in particular, we have that

\[
p_2(n_2) = \sum_{s_1} q(s_1, n_2), \tag{2.6}
\]
in contrast to Eq.\(2.2\). However, the quasi-probability can be negative, which we regard as an indication of quantum-mechanical behaviour. When non-negative, it is our candidate expression for the path probabilities in the double-slit experiment and Eq.\(2.6\) is then the statement that the interference pattern probability \textit{can} be regarded as the sum of two path probabilities.

The quasi-probability Eq.\(2.5\) has a simple relation to the standard quantum-mechanical two-time probability Eq.\(2.2\), namely,

\[
q(s_1, n_2) = p_{12}(s_1, n_2) + \text{Re} D(s_1, n_2 | -s_1, n_2), \tag{2.7}
\]

where the quantity

\[
D(s_1, n_2 | s_1', n_2) = \text{Tr} \left( E_{n_2}(t_2) P_{s_1}(t_1) \rho P_{s_1'}(t_1) \right), \tag{2.8}
\]
is the decoherence functional, and is a measure of the interference between different paths in the interferometer. (Here we employ the mathematical machinery of the decoherent histories approach to quantum theory \[18\,23\]). Note that this interference term vanishes when the NSIT condition Eq.\(2.4\) holds. By summing Eq.\(2.7\) over \(s_1\), we obtain

\[
p_2(n_2) = \sum_{s_1} p_{12}(s_1, n_2) + 2 \text{Re} D(s_1, n_2 | -s_1, n_2). \tag{2.9}
\]
(Noting that \( \text{Re}D(s_1, n_2|s_1, n_2) \) is in fact independent of \( s_1 \), since \( s_1 \) takes only values \( \pm 1 \)).

This relation shows precisely how non-zero interference prevents the sum rules from being satisfied. Furthermore, one can see immediately how the negativity of the quasi-probability may be related to the interference pattern. The right-hand side of Eq. (2.9) consists of a positive term (essentially the mean size of the interference pattern) plus an interference term which can be positive (constructive interference) or negative (destructive interference).

From Eq. (2.7), one can see that the quasi-probability is negative if \( \text{Re}D(s_1, n_2|s_1, n_2) \) is negative and sufficiently large. Hence negative quasi-probability is closely related to destructive interference.

We now sketch the relationship between the quasi-probability and the LG inequalities. For simplicity, we first consider the case in which the projections at both times are two-valued and take the form \( P_s = (1 + s\hat{Q})/2 \), for a dichotomic variable \( \hat{Q} \). (We use hats to denote operators only when the difference between classical and quantum versions is not obvious, which in practice affects only the variable \( Q \)). The quasi-probability is then conveniently expanded in terms of its moments,

\[
q(s_1, s_2) = \frac{1}{4} \left( 1 + \langle \hat{Q}_1 \rangle s_1 + \langle \hat{Q}_2 \rangle s_2 + C_{12} s_1 s_2 \right),
\]

where the correlation function \( C_{12} \) is given by,

\[
C_{12} = \frac{1}{2} \langle \hat{Q}_1 \hat{Q}_2 + \hat{Q}_2 \hat{Q}_1 \rangle,
\]

and we use the notation \( \hat{Q}_1 = \hat{Q}(t_1), \hat{Q}_2 = \hat{Q}(t_2) \). The conditions

\[
q(s_1, s_2) \geq 0,
\]

are then precisely a set of four two-time LG inequalities, written in quantum form. Macrorealistically, they correspond to the situation in which we make measurements of variables \( Q_1 \) and \( Q_2 \) at times \( t_1 \) and \( t_2 \) to determine the averages \( \langle Q_1 \rangle, \langle Q_2 \rangle \) and the correlator \( C_{12} = \langle Q_1 Q_2 \rangle \). For a macrorealistic theory, a joint probability for \( Q_1 \) and \( Q_2 \) exists which implies that the inequalities

\[
\langle (1 + s_1 Q_1)(1 + s_2 Q_2) \rangle \geq 0,
\]

must hold. Expanded out, this yields the LG inequalities,

\[
1 + s_1 \langle Q_1 \rangle + s_2 \langle Q_2 \rangle + s_1 s_2 C_{12} \geq 0.
\]
These are clearly necessary conditions for macrorealism. They are also sufficient since the inequalities themselves, when satisfied and multiplied by $\frac{1}{4}$, are the probabilities for the two histories matching the measured data.

The LG inequalities Eq. (2.14) define a version of macrorealism christened weak macrorealism in Ref. [4]. This is to contrast it with alternative definitions characterized by the NSIT condition Eq. (2.4) being satisfied, which is referred in Ref. [4] to as strong macrorealism. These two conditions have a clear logical relationship, namely that the NSIT condition implies the LG inequalities but not conversely. However, this logical relationship no longer holds when we go beyond dichotomic variables [6], as is the case in the triple-slit experiment considered below.

Returning now the case in which measurements are made at the screen using the many-valued projector $P_n$, we can easily relate this to the dichotomic case by picking a fixed value of $n$ and defining a dichotomic variable $Q(n) = 2P_n - \mathbb{1}$, where $\mathbb{1}$ is the identity operator. The set of LG inequalities Eq. (2.14) in which $Q_2$ is replaced by the set of dichotomic variables $Q_2(n)$ is then readily seen to be equivalent to the requirement,

$$q(s_1, n_2) \geq 0.$$ (2.15)

This set of relations is therefore the natural generalization of the standard LG inequalities, generalized to many-valued variables at the second time [6].

Turning now to measurement procedures, the standard two-time LG inequalities are tested by measuring $\langle Q_1 \rangle$, $\langle Q_2 \rangle$ and the correlator $C_{12}$ in three different experiments, where the experiment measuring the correlator must be done non-invasively [4, 24–27]. This is typically achieved using ideal negative measurements but other methods exist (see for example Refs. [28–30]). This procedure can then be repeated for many choices of the dichotomic variables $Q_2(n)$ and the quasi-probability $q(s_1, n_2)$ can be constructed. However, it is not hard to see that there is a more direct way which is equivalent. This is to note from Eqs. (2.7), (2.9), that the interference term may be eliminated and we find the convenient formula,

$$q(s_1, n_2) = p_{12}(s_1, n_2) + \frac{1}{2} \left( p_2(n_2) - \sum_{s'_1} p_{12}(s'_1, n_2) \right).$$ (2.16)

This quantity can therefore be determined by measuring $p_{12}(s_1, n_2)$ using an ideal negative measurement and measuring $p_2(n_2)$ in a separate experiment. Furthermore, although this
formula is derived using quantum mechanics, it can be postulated as a candidate probability in purely macrorealistic terms. For suppose we first measure $p_{12}(s_1, n_2)$ and discover it fails to satisfy the sum rules, i.e. to match $p_2(n_2)$ when summed over $s_1$. One could simply then try to modify the sequentially measured formula by a term proportional to the sum rule violation, in such a way as to ensure that both marginals $p_1(s_1)$ and $p_2(n_2)$ can be matched. Eq. (2.16) is the obvious guess through which this may be accomplished. This method of determining $q(s_1, n_2)$ is in practice probably the easiest to implement experimentally, since as we shall see in the next section, it can avoid the issue of overall normalization.

As we shall see in Section 4, the quasi-probability may also be measured more directly, using a pair of sequential measurements in which the first one is weak [13] (or more generally, ambiguous, as we discuss later). For such measurements opinion remains divided as to whether weak measurements really meet the NIM requirement in LG tests [7, 31], and we will not assume that here.

III. EXPLICIT CALCULATION FOR THE DOUBLE SLIT EXPERIMENT

We now apply the formalism to developed in the previous section for specific initial states for the double-slit experiment. We choose an initial state

$$|\psi\rangle = \sum_s \alpha_s |\psi_s\rangle,$$

(3.1)

which represents the state immediately after the particle has impinged on the slits, where $\sum_s |\alpha_s|^2 = 1$. The states $|\psi_\pm\rangle$ are gaussians strongly concentrated at $x = \pm L$,

$$\psi_\pm(x) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} \exp\left(-\frac{(x \mp L)^2}{4\sigma^2}\right)$$

(3.2)

and are approximate eigenstates of $P_{s_1}$. We readily find

$$q(s_1, n_2) = \text{Re} \sum_s \alpha_{s_1}^* \alpha_{s_1} \langle \psi_s(\tau)|E_{n_2}|\psi_{s_1}(\tau)\rangle$$

$$= |\alpha_{s_1}|^2 \langle \psi_{s_1}(\tau)|E_{n_2}|\psi_{s_1}(\tau)\rangle + \text{Re} \sum_{s \neq s_1} \alpha_{s_1}^* \alpha_{s_1} \langle \psi_s(\tau)|E_{n_2}|\psi_{s_1}(\tau)\rangle,$$

(3.3)
where for convenience we take \( t_1 = 0 \) and \( t_2 = \tau \). (There is only one term in the sum, namely \( s = -s_1 \), but the form given generalizes to the three-slit case). We also find,

\[
p_{12}(s_1, n_2) = |\alpha_{s_1}|^2 \langle \psi_{s_1}(\tau) | E_{n_2} | \psi_{s_1}(\tau) \rangle, \quad (3.4)
\]

\[
p_2(n_2) = \sum_{s,s_1} \alpha_{s}^{*} \alpha_{s_1} \langle \psi_{s}(\tau) | E_{n_2} | \psi_{s_1}(\tau) \rangle. \quad (3.5)
\]

In all these expressions, \( |\psi(\tau)\rangle = \exp(-\frac{i}{\hbar}H\tau)|\psi\rangle \), where \( H \) is the free particle Hamiltonian.

We now make the simplification that the projections at the screen are onto extremely narrow ranges of size \( \Delta \) so that \( E_n \) is approximated by \( \Delta |x\rangle \langle x| \) where \( x = n\Delta \). This means that

\[
\langle \psi_{s}(\tau) | E_{n_2} | \psi_{s_1}(\tau) \rangle \approx \Delta \psi_{s}^{*}(x,\tau)\psi_{s_1}(x,\tau). \quad (3.6)
\]

For simplicity we take the initial wave functions \( \psi_{s}(x) \) to be approximated by \( \delta \)-functions \( \delta(x - sL) \), up to normalization, which are readily found to evolve into

\[
\psi_{s}(x,\tau) = N_{\tau} \exp \left( i\frac{m(x - sL)^2}{2\hbar \tau} \right). \quad (3.7)
\]

The normalization factor \( N_{\tau} \) will slowly decay to zero for large \( |x| \) in a more exact treatment but the explicit form is not required in what follows. We also take

\[
\alpha_{+} = \cos \phi \ e^{i\theta_{+}}, \quad \alpha_{-} = \sin \phi \ e^{i\theta_{-}}, \quad (3.8)
\]

and define \( \theta = \theta_{+} - \theta_{-} \). It is convenient to define quasi-probability densities \( q(s_1, x) = q(s_1, n_2)/\Delta \) (estimating the risk of notational confusion to be small), and we get

\[
q(+, x) = \frac{1}{2} |N_{\tau}|^2 \left( 1 + \cos 2\phi + \sin 2\phi \cos \left( \frac{2mxL}{\hbar \tau} - \theta \right) \right), \quad (3.9)
\]

\[
q(-, x) = \frac{1}{2} |N_{\tau}|^2 \left( 1 - \cos 2\phi + \sin 2\phi \cos \left( \frac{2mxL}{\hbar \tau} - \theta \right) \right). \quad (3.10)
\]

The screen probability density is

\[
p_{2}(x) = q(-, x) + q(+, x) \quad (3.11)
\]

\[
= |N_{\tau}|^2 \left( 1 + \sin 2\phi \cos \left( \frac{2mxL}{\hbar \tau} - \theta \right) \right). \quad (3.12)
\]

We also get

\[
p_{12}(s_1, x) = \frac{1}{2} |N_{\tau}|^2 (1 + s_1 \cos 2\phi), \quad (3.13)
\]
and the mean of the interference pattern is,
\[ \sum_{s_i} p_{12}(s_1, x) = |N_t|^2. \] (3.14)
These relations are all consistent with Eq. (2.9), as expected.

To explore the connection between the sign of the quasi-probabilities and the interference pattern, first note that only one of \( q(+, x) \) and \( q(−, x) \) can be negative, since they sum to a positive number. It is then convenient to examine the quantity,
\[ q(+, x)q(−, x) = \frac{1}{4} |N_t|^4 \left[ \left( 1 + \sin 2\phi \cos \left( \frac{2mxL}{\hbar \tau} - \theta \right) \right)^2 - \cos^2 2\phi \right], \] (3.15)
which is negative if either one is negative. Comparing with Eq. (3.12), it is then clear that the only way for either quasi-probability to be negative is for the interference pattern to show destructive interference, i.e. the interference term in Eq. (3.12) is negative, that is
\[ \sin 2\phi \cos Y < 0, \] (3.16)
where
\[ Y = \frac{2mxL}{\hbar \tau} - \theta. \] (3.17)
Plots of the parameter ranges for which there is destructive interference and LG violation are shown in Figure 2.

The plots show the following features. The most important feature is that LG violation, negativity of Eq. (3.15), is always accompanied by destructive interference. But the converse is not true in general – there are significant regions where there is destructive interference but no LG violation. This means that it is in fact often possible to assign probabilities to the paths in a double-slit experiment even in the face of destructive interference. This feature is also shown plotted differently in Figure 3.

However, there are special parameter values for which LG violation and destructive interference are more tightly related. First, for values of \( \phi \) in the neighbourhood of \( n\pi/2 \), for \( n = 0, ±1, ±2 \), the regions of destructive interference with no LG violation are very small. Hence there is an approximate coincidence. (Although note that both the quasi-probabilities and interferences are close to zero for these values.)

Second, for \( Y = 0 \) and \( Y = \pi \), there are significant ranges of \( \phi \) for which destructive interference coincides entirely with LG violation. The analysis here of LG violations and
FIG. 2: The grey/black rectangles show the regions in the parameter space \((\phi, Y)\) for which there is destructive interference (and no destructive interference in the white rectangles). In the black regions there is also LG violation, but no violation in the grey regions. The figure clearly shows that regions of LG violation correspond to destructive interference but destructive interference can occur without LG violation for a wide range of parameters. LG violation and destructive interference can however coincide for special parameter choices.

destructive interference is then in fact mathematically the same as the analysis of interferences in the MZ interferometer considered by Pan [8] who found a perfect coincidence between LG violations and destructive interference. This coincidence of course follows from a quantum-mechanical argument but a plausible macrorealistic argument that destructive interference implies LG violation in this case was also given. This was then argued to imply that the non-invasiveness assumption made in LG tests is not in fact required, since the LG violation is deduced indirectly from a single final measurement. This is an appealing conclusion which avoids one of the most fraught issues of LG tests. Here, this argument only applies for very specific parameter values so we will stay with the usual assumption that a non-invasive measurement is performed at the first time in order to check for LG violations. The degree of LG violation and destructive interference are not simply related. The
FIG. 3: A plot of the LG violation discriminant Eq. (3.15) as a function of $Y$ (up to an overall factor) and of the size of the interference term $\sin(2\phi)\cos(Y)$ in Eq. (3.12), both for $\phi = 0.5$ (a typical value). There are clear ranges of $Y$ (between the pairs of vertical lines) for which there is destructive interference but no LG violation.

The maximum LG violation occurs when the destructive interference is at about half its maximum. On the other hand there are discrete values of $\phi$ for which the LG inequalities are satisfied for all $Y$ but these in fact correspond to maximal destructive interference. For example, this happens at $\phi = \pi/4$ and $Y = \pi$ and this is shown more explicitly in Figure 4. The two quasi-probabilities are actually zero at this point, which means that maximal destructive interference is not in fact obtained through LG violation here, but through the two contributing quasi-probabilities both being zero. However, this is an atypical point and the surrounding parameter ranges give LG violation and destructive interference.

A question remains as to the absolute size of any of the LG violations obtained in this situation. The quasi-probability Eq. (2.5) is bounded from below by $-1/8$. This is the Lüders bound discussed later and corresponds to a lower bound of $-1/2$ in a LG violation. To see how close the LG violations in the double-slit experiment are, we would need full details of the normalization, which is somewhat lengthy to describe. Instead, some sense of the size of the violations may be obtained using the following dichotomization process.
FIG. 4: A plot of the LG violation discriminant Eq. (3.15) and the size of the interference term in Eq. (3.12) for the special value $\phi = \pi/4$. The destructive interference reaches its maximum value but the LG inequalities are always satisfied for all $Y$.

We post-select onto a finite region of the screen, which is divided into two regions labeled by $s_2 = \pm 1$. Properly normalized quasi-probabilities $q(s_1, s_2)$ are then obtained from those obtained above by dividing by the probability of the finite region and all dependence on the normalization factor $N_\tau$ drops out. A convenient choice of post-selection region is to take $s_2 = +1$ to be $-\pi/2 < Y < \pi/2$ and $s_2 = -1$ to be $\pi/2 < Y < 3\pi/2$, i.e. the light and dark regions of the interference pattern where $\cos Y$ is positive or negative respectively. We then readily find that the properly normalized post-selected quasi-probability is

$$q(s_1, s_2) = \frac{1}{4} \left( 1 + \cos(2\phi)s_1 + \frac{2}{\pi} \sin(2\phi)s_2 \right).$$

This has lower bound of about $-0.05$ which is about 40% of the Lüders bound of $-0.125$. Although note that the derivation of the Lüders bound (in Ref. [12] for example) does not obviously apply to the post-selection situation so this result is only indicative. It does however indicate that the LG violation is not insignificant.

This dichotomization process may also be relevant to experimental tests, since any measurement can measure at best coarse grainings of the probability density $p_2(x)$ of arriving
at the screen at point $x$. Focusing on light versus dark patches is clearly a convenient coarse graining.

IV. MEASUREMENT OF WHICH SLIT THE PARTICLE WENT THROUGH

We now examine a related but different aspect of the double-slit experiment. So far we have been interested in a LG experiment which constitutes an indirect determination of whether or not one can assign probabilities to the paths. However, it is natural to consider the different but related question as to the probability obtained by actually measuring which slit the particle went through. One can then ask how this probability is related to the one obtained through a LG test and also examine how this measurement affects the interference pattern as the accuracy of the measurement is varied. This question has certainly been considered before [32], and at least one experiment has been done [33]. However, the formalism developed here and earlier [12] provides a concise account of the situation and furthermore shows that the quasi-probability description of the situation using Eq.(2.5) is one of a family of similar possibilities. Note however that this is no longer a LG test due to the question mark mentioned earlier as to whether such measurements at the slit meet the requirement of non-invasiveness, even if weak.

The essence of earlier approaches to this problem is to carry out a measurement at the slits which is weaker than a projective measurement, and therefore imperfect, but still gives a reasonably good idea as to which slit the particle went through. A convenient way to approach this problem is to use ambiguous measurements [34, 35] which provide a continuum of measurement strengths mediating between standard projective measurements and weak measurements [36]. The idea is that when a definite value $s = \pm 1$ is measured, the imperfection of the measurement means that the measurement yields a value $\alpha = \pm 1$ with conditional probability $c_{\alpha s}$. Ambiguous measurements are therefore described by a positive operator-valued measure,

$$F(\alpha) = \sum_s c_{\alpha s} P_s.$$  \hspace{1cm} (4.1)

For a single time measurement, from the experimentally measured probability $p(\alpha) = \text{Tr}(F_\alpha \rho)$ the desired probability of $s$, $\tilde{p}(s)$ is recovered by inversion,

$$\tilde{p}(s) = \sum_\alpha d_{\alpha s} p(\alpha),$$  \hspace{1cm} (4.2)
where $d_{sa}$ is the inverse of $c_{as}$. This procedure is essentially trivial for a single-time measurement but becomes non-trivial when used as a pair of sequential measurements in which the first one is ambiguous. What happens is that the weakness of the measurements compared to projective measurements reduces the degree to which interference effects contribute.

The relevant calculations are described in detail in Ref. [12]. The conditional probability $c_{as}$ is taken to be

$$c_{as} = \frac{1}{2}(1 + \varepsilon) \delta_{as} + \frac{1}{2}(1 - \varepsilon) \delta_{a,-s} \quad (4.3)$$

where $\varepsilon$ ranges from 0 to 1, where $\varepsilon = 1$ corresponds to a projective measurement and small values correspond to a weak measurement. The ambiguously measured joint probability density for measurements at both the slits and the screen is then found to be,

$$\tilde{p}_\varepsilon(s_1, x) = (1 - \sqrt{1 - \varepsilon^2}) p_{12}(s_1, x) + \sqrt{1 - \varepsilon^2} q(s_1, x). \quad (4.4)$$

This object therefore mediates continuously between the sequentially measured probability Eq.(2.2) for projective measurements and the quasi-probability Eq.(2.5) for weak measurements. It may in fact be negative since $q(s_1, x)$ can be negative. This is a reflection of the way in which this object is measured and constructed which only guarantees non-negativity at a macrorealistic level.

Inserting explicit values for $p_{12}(s_1, x)$ and $q(s_1, x)$ for the double slit experiment, we have

$$\tilde{p}_\varepsilon(s_1, x) = \frac{1}{2}|N_t|^2 \left(1 + \sqrt{1 - \varepsilon^2} \left[s_1 \cos 2\phi + \sin 2\phi \cos \left(\frac{2mxL}{\hbar \tau} - \theta\right)\right]\right). \quad (4.5)$$

Summing over $s_1$ we find that the screen probability with ambiguous measurement at the slits is,

$$\tilde{p}_\varepsilon(x) = |N_t|^2 \left(1 + \sqrt{1 - \varepsilon^2} \sin 2\phi \cos \left(\frac{2mxL}{\hbar \tau} - \theta\right)\right). \quad (4.6)$$

As expected, by comparing with the screen probability without a measurement at the slits Eq.(3.12) we see that the intensity of the interference pattern is suppressed by a factor of $\sqrt{1 - \varepsilon^2}$, which varies from zero for projective measurements to close to 1 for very weak measurements.

The issue now is simply to examine the relationship between the suppression factor $\sqrt{1 - \varepsilon^2}$, and the probability $p = (1 + \varepsilon)/2$ of a faithful measurement. We first qualitatively look at the interference pattern for values of $\phi$ such that $\sin(2\phi)$ is maximised. In this case the screen pattern is given by

$$\tilde{p}_\varepsilon(x) = |N_t|^2 (1 + \sqrt{1 - \varepsilon^2} \cos(y)), \quad (4.7)$$
FIG. 5: The interference pattern seen at the screen when weakly measuring the particle path for a) 50% b) 75% and c) 90% certainty of measuring the slit a particle has gone through.

where $y$ is defined in Eq. (3.17). Figure 5 shows what the interference pattern would look like with increasing certainty as to which slit the particle went through. Even with 90% certainty of knowing which slit the particle has gone through, the interference pattern can still be distinguished.

For a more quantifiable measure we consider the trough to peak ratio $r$ of the interference pattern which is

$$r = \frac{1 - \sqrt{1 - \varepsilon^2}}{1 + \sqrt{1 - \varepsilon^2}}.$$  \hfill (4.8)

A plot of this against the degree of certainty $p$ is shown in Figure 6. Clearly the interference pattern can be maintained to a large degree with relatively high levels of certainty. Even at 99% measurement certainty the peak to trough ratio is 0.67 which should be visible to the eye. (Interestingly, the same result for 99% certainty is obtained in Ref. [32] despite using a different method of modelling the situation).

V. THE TRIPLE SLIT EXPERIMENT

We consider now the generalization of the approach described in Sections 2 and 3 to the triple-slit experiment [37]. We find what is new here is that there are three different types of interference terms. There is again a discussion of the relationship between LG violation and destructive interference, but this relationship is more fluid than in the double-slit case, except for certain parameter values. More importantly, the triple-slit experiment
FIG. 6: A comparison between the peak-trough ratio $r$ of the screen probability and the measure of certainty $p$ in determining which slit the particle went through. The minimum value for $p$ of 0.5 corresponds to $\epsilon = 0$. A high degree of certainty can be reached whilst maintaining the interference pattern – the dashed line corresponds to a certainty of 99% which corresponds to a ratio of 0.67.

provides testable examples of the new types of MR conditions that arise once we go beyond dichotomic variables to variables with three or more values. In particular, as argued in Ref. [6], the relationship between NSIT conditions and LG inequalities is much richer than in the dichotomic case. Also, the correlators for many-valued variables can be measured in more than one way, and with some methods, there is the possibility of a violation of the Lüders bound (the mathematical parallel to the Tsirelson bound in Bell experiments).

A. Interferences and quasi-probabilities

The formalism developed so far generalizes very readily to the triple slit. We choose the three slits to be located at $x = \pm L$ and $x = 0$. Alternatives at time $t_1$ are denoted by $n_1$ which may take values $-1, 0, 1$ and measurements at that time implemented through the projector $E_{n_1}$ and there is again a measurement $E_{n_2}$ at the screen. The two-time LG
inequalities are simply
\[ q(n_1, n_2) \geq 0 \] (5.1)
where the quasi-probability \( q(n_1, n_2) \) is the trivial generalization of Eq.(2.5). The two-time measurement probability \( p_{12}(n_1, n_2) \) and quasi-probability \( q(n_1, n_2) \) are again simply related and we have
\[ q(n_1, n_2) = p_{12}(n_1, n_2) + \sum_{n_1', n_2'} \text{Re}D(n_1, n_2|n_1'n_2'). \] (5.2)

The probability at the second time can be written as
\[ p_2(n_2) = \sum_{n_1} p_{12}(n_1, n_2) + \sum_{n_1, n_1'} \text{Re}D(n_1, n_2|n_1'n_2'). \] (5.3)

In the double-slit case there was just one interference term. In the triple-slit case there are three for fixed \( n_2 \).

We take the state just after the slits to be
\[ |\psi\rangle = \sum_n \alpha_n |\psi_n\rangle, \] (5.4)
where \( |\psi_\pm\rangle \) have the form Eq.(3.2) and \( |\psi_0\rangle \) has the same form but with \( L = 0 \). A convenient form for the coefficients \( \alpha_n \), which ensures the proper normalization is
\[ \alpha_+ = e^{i\chi_+} \sin \theta \cos \phi, \]
\[ \alpha_- = e^{i\chi_-} \sin \theta \sin \phi, \]
\[ \alpha_0 = \cos \theta. \] (5.5)

Given this parametrisation the value of the screen probability density \( p_2(x) = |\psi(x, \tau)|^2 \) is found to be
\[ p_2(x) = |N_t|^2 \left[ 1 + 2 \cos \theta \sin \theta \cos \phi \cos(X_+) + 2 \cos \theta \sin \theta \sin \phi \cos(X_-) \right. \]
\[ \left. + 2 \sin^2 \theta \cos \phi \sin \phi \cos(X) \right], \] (5.6)
where
\[ X_+ = \frac{m}{2\hbar} (L^2 - 2Lx) + \chi_+ \] (5.7)
\[ X_- = \frac{m}{2\hbar} (L^2 + 2Lx) + \chi_- \] (5.8)
\[ X = \frac{2mLx}{\hbar} + \chi_- - \chi_+ = X_- - X_+. \] (5.9)
This may be written in more condensed notation as

\[ p_2(x) = |N_t|^2\left[1 + 2I_{0,+} + 2I_{-,0} + 2I_{-,+}\right], \quad (5.10) \]

where,

\[ I_{0,+} = \sin \theta \cos \theta \cos \phi \cos (X_+), \quad (5.11) \]
\[ I_{-,0} = \sin \theta \cos \theta \sin \phi \cos (X_-), \quad (5.12) \]
\[ I_{-,+} = \sin^2 \theta \cos \phi \sin \phi \cos (X). \quad (5.13) \]

The interference terms \( I_{n_1,n_1'} \) are related to the off-diagonal terms of the decoherence functional in Eq.\((5.2)\) by

\[ \text{Re} D(n_1, n_2| n_1' n_2) = |N_t|^2 I_{n_1,n_1'}. \quad (5.14) \]

(And note that this notation differs from that in Ref.\([6]\) by a factor of \( |N_t|^2 \).)

The form of \( p_{12}(n_1, x) \), using similar reasoning to the double-slit case, results in

\[ p_{12}(n_1, x) = |\alpha_{n_1}|^2 |N_t|^2. \quad (5.15) \]

Calculating the quasi-probabilities for the triple slit with the \( X_\pm \) substitution results in

\[ q(+, x) = |N_t|^2 \left[ \sin^2 \theta \cos^2 \phi + I_{0,+} + I_{-,+}\right], \quad (5.16) \]
\[ q(-, x) = |N_t|^2 \left[ \sin^2 \theta \sin^2 \phi + I_{-,0} + I_{-,+}\right], \quad (5.17) \]
\[ q(0, x) = |N_t|^2 \left[ \cos^2 \theta + I_{0,+} + I_{-,0}\right], \quad (5.18) \]

and note that the sum of these three yields \( p_2(x) \) as expected.

These three quasi-probabilities are determined experimentally using three dichotomizations of \( n_1 \) at \( t_1 \) and then using the formula Eq.\((2.16)\). For example, to determine \( q(+, x) \), we consider the dichotomic variable

\[ \hat{Q} = 2E_+ - \mathbb{1}, \quad (5.19) \]

and do non-invasive measurements to determine the sequential measurement probability \( p_{12}^{\hat{Q}}(s_1, x) \). This together with the probability \( p_2(x) \) permits the determinaton via Eq.\((2.16)\) of the quasi-probability \( q(s_1, x) \), and setting \( s_1 = +1 \) yields the desired result. Similarly for the other two.
The screen probability Eq.\((5.7)\) involves a sum of all three interference terms but each of the three quasi-probabilities \(q(n_1, x)\) involves only two interference terms. This means that, unlike the double-slit case, there is no general logical relationship between destructive interference and violation of the LG inequalities,

\[
q(n_1, x) \geq 0,
\]
and indeed they can behave quite independently. There are parameter ranges for which LG violation is accompanied by destructive interference, as in the double-slit case. There are parameter ranges which are the opposite to that case: LG violation but no destructive interference. The latter case arises because \(p_2(x)\) is now a sum over three quasi-probabilities, two of which can cancel each other out if one is negative, leaving a third one which can exhibit either constructive or destructive interference. It is also possible to find parameters for which LG violation and destructive interference perfectly coincide. This lack of clear relationship is simply due to the fact that destructive interference alone for the triple slit experiment is a single and very coarse-grained characteristic of the system compared to the more detailed description provided by the set of LG inequalities.

**B. Two-time NSIT conditions in the Triple Slit Experiment**

More precise statements may be made by focusing in on NSIT conditions. In Section 2 we noted that the NSIT condition Eq.\((2.4)\) has a clearly logical connection to the two-time LG inequalities, namely the former implies the latter, but not conversely. This is because the NSIT condition implies that the single interference term encountered there must vanish but the LG inequalities require only that it is not too large.

However, this was for measurement of a single dichotomic variable at the first time. For the triple-slit experiment, in which we are in effect measuring a three-valued variable at the first time, a more complicated relationship arises. For a system taking three values at the first time, the natural analogue of the NSIT condition Eq.\((2.4)\) is,

\[
\sum_{n_1} p_{12}(n_1, n_2) = p_2(n_2).
\]

We then readily see from the above that in the triple-slit experiment this means that the sum of all three interference terms must vanish,

\[
I_{-,0} + I_{0,+} + I_{-,+} = 0.
\]
That is, there is neither constructive nor destructive interference. However, this clearly does not imply that all the LG inequalities are satisfied, since this requires that the sums of pairs of interferences terms are sufficiently small.

It is of interest to illustrate the parameter ranges that there is LG violation but with the NSIT conditions Eq. (5.21) satisfied. The NSIT condition may be written explicitly as,

\[
\cos \theta \sin \theta \cos \phi \cos(X_+) + \cos \theta \sin \theta \sin \phi \cos(X_-) + \sin^2 \theta \sin \phi \cos \phi \cos(X) = 0. \quad (5.23)
\]

This condition can be rearranged as follows

\[
\tan \theta = -\frac{\cos \phi \cos(X_+) + \sin \phi \cos(X_-)}{\sin \phi \cos \phi \cos(X)}. \quad (5.24)
\]

which can be readily substituted into the forms for the quasiprobabilities. This results in quasiprobabilities of the form

\[
q(\pm, x) \propto \sin^2 \theta \left( \cos^2 \phi + \cos \phi \sin \phi \cos(X) \left( 1 - \frac{1}{1 + \tan \phi \cos(X)} \right) \right), \quad (5.25)
\]
\[
q(-, x) \propto \sin^2 \theta \left( \sin^2 \phi + \cos \phi \sin \phi \cos(X) \left( 1 - \frac{1}{1 + \cot \phi \cos(X)} \right) \right), \quad (5.26)
\]
\[
q(0, x) \propto \cos^2 \theta \left( 1 - \left[ \frac{\cos \phi \cos(X_+) + \sin \phi \cos(X_-)}{\sin \phi \cos \phi \cos(X)} \right]^2 \right). \quad (5.27)
\]

The parameter ranges for which at least one of these is violated are shown in Figure 7. There are clearly substantial regions of LG violation even though the NSIT condition is satisfied.

Examples of this form, in which LG violation is observed when a NSIT condition holds, have been discovered previously and observed experimentally \[35, 38, 39\]. A general analysis of this initially surprising phenomenon was given in Ref. \[6\]. The key point is that for situations such as the triple-slit experiment, there is not just one NSIT condition. The other NSIT conditions may be found by considering all possible dichotomic variables at the first time, which we denote \(\hat{Q}(n_1)\) and are given by

\[
\hat{Q}(n_1) = 2E_{n_1} - \mathbb{I}, \quad (5.28)
\]

where \(\mathbb{I}\) denotes the identity operator. Each choice of \(\hat{Q}\) produces a two-time probability \(p_{12}^Q(s_1, n_2)\) for \(s_1 = \pm 1\) and if we require that each satisfies its own NSIT condition,

\[
\sum_{s_1} p_{12}^Q(s_1, n_2) = p_2(n_2), \quad (5.29)
\]
FIG. 7: The shaded region of this parameter space shows the regions where the quasiprobabilities are negative for the triple slit whilst the overall NSIT condition is met. In this figure $X_+ = 0.001$. Hence LG violations are still possible when the overall NSIT condition is met.

we then find that the interference terms must satisfy,

$$I_{0,+} + I_{-,+} = 0,$$  \hspace{1cm} (5.30)  

$$I_{-,0} + I_{-,+} = 0,$$  \hspace{1cm} (5.31)  

$$I_{-,0} + I_{0,+} = 0,$$  \hspace{1cm} (5.32)  

which actually imply Eq. (5.22). So there are in fact three independent NSIT conditions (for fixed $n_2$) and if any three of the conditions Eq. (5.22), Eq. (5.30)-(5.32) are satisfied than all interferences terms are zero and all NSIT conditions hold. This means that if all NSIT conditions hold then the LG inequalities must be satisfied, in parallel with the double-slit case, but if only some NSIT conditions hold, then some of the LG inequalities can still be violated.
C. Lüders Bound Violations

The quasi-probability Eq.\,(2.5) has lower bound $-1/8$ and correspondingly the maximum violation of the two-time LG inequalities Eq.\,(1.2) is $-1/2$. This is the Lüders bound and is the maximal violation possible for projective measurements of a dichotomic variable $Q$ (Lüders measurements) and coincides numerically with the Tsirelson bound in Bell experiments. However, for systems with three or more levels, there are different macrorealistically equivalent methods of measuring the correlators which permit violations of the Lüders bound.

In the usual method involving Lüders measurements of say, a three-level system, we measure the dichotomic variable defined by

$$\hat{Q} = \sum_n \epsilon(n) E_n,$$  \hspace{1cm} (5.33)

for some coefficients $\epsilon(n) = \pm 1$ with at least one minus and one plus. $\hat{Q}$ has eigenvalues $\pm 1$ but unlike the dichotomic case for two-level systems, its spectrum is now degenerate. The resulting correlation function has the form Eq.\,(2.11) and is referred to as the Lüders correlator, denoted $C_{12}^L$. It may be written in terms of the quasi-probability as,

$$C_{12}^L = \sum_{n_1, n_2} \epsilon(n_1)\epsilon(n_2) q(n_1, n_2).$$  \hspace{1cm} (5.34)

(Note this formula refers to a situation in which there are three-valued measurements at the second time also, but what follows applies to a dichotomic measurement at the second time also). We may instead to do a set of finer-grained measurements modelled by the projectors $E_n$ and determine the sequential measurement probability $p_{12}(n_1, n_2)$. These so-called von Neumann measurements yield the von Neumann correlator,

$$C_{12}^{vN} = \sum_{n_1, n_2} \epsilon(n_1)\epsilon(n_2) p_{12}(n_1, n_2).$$  \hspace{1cm} (5.35)

The two methods are macrorealistically equivalent but give different results in quantum mechanics, and in particular we find,

$$C_{12}^{vN} = C_{12}^L - \sum_{n_1 \neq n_1'} \sum_{n_2} \epsilon(n_1)\epsilon(n_2) \Re D(n_1, n_2|n_1', n_2)$$  \hspace{1cm} (5.36)

as is readily shown. LG inequalities constructed from $C_{12}^{vN}$, such as

$$1 + \langle Q_1 \rangle + \langle Q_2 \rangle + C_{12}^{vN} \geq 0,$$  \hspace{1cm} (5.37)
need not satisfy the Lüders bound of $-1/2$ on the right-hand side and may in fact violate the inequality up to the algebraic maximum. The underlying reason for the violation is to do with interference terms between the states in the degenerate subspace of $\hat{Q}$. See Refs. [6, 44] for further discussion of the details and the interpretation of Lüders bound violations.

Here we show that such a violation is possible in the triple slit experiment. We take a dichotomic variable at the slits defined by Eq. (5.19). It may be shown that the von Neumann version of the LG inequality corresponds to replacing, for example, the quasi-probability Eq. (5.16), with

$$q^{vN}(+, x) = |N_t|^2 \left[ \sin^2 \theta \cos^2 \phi + I_{0,+} + I_{-,+} - I_{-,0} \right]. \quad (5.38)$$

(See for example Eq. (6.10) in Ref. [6], from which one can see that the interference term in Eq. (5.36) corresponds to the term $I_{-,0}$). To show that Eq. (5.38) may be more negative than the Lüders bound of $-1/8$ requires a more detailed account of the normalization factors and dichotomization of the screen variable $x$, since the bound is sensitive to the overall scale of the LG inequalities (unlike most of the features we have looked at so far). As noted before in the double-slit case this is somewhat complicated, and turns out to be a lot more complicated in the triple-slit case. We briefly report here that we have carried out this detailed calculation and confirm that a Lüders violation is readily found for various parameter ranges, although we do not give these details here. Instead, we will display a paired-down version of the problem, along the lines described in Ref. [44], which conveniently avoids having to spell out the details of the normalization.

The idea is to restrict parameters so that the original LG inequality $q(+, x) \geq 0$ with Lüders measurements is always satisfied, hence within this restricted parameter set, the Lüders bound is zero, which is independent of overall scale. A violation of $q^{vN}(+, x) \geq 0$ within the same parameter set therefore signals a violation of the Lüders bound. In fact one simple way to approach this is to restrict to parameters for which the NSIT condition associated with $\hat{Q}$ is satisfied exactly, which means that $I_{0,+} + I_{-,+} = 0$. This is easily achieved by taking $\phi = \pi/2$. We then have

$$q^{vN}(+, x) = |N_t|^2 \left[ \sin^2 \theta \cos^2 \phi - \sin \theta \cos \theta \sin \phi \cos(X_-) \right], \quad (5.39)$$

where we have inserted the explicit value of $I_{-,0}$. Violations of $q^{vN}(+, x) \geq 0$ are then easily
found. For example, \( \phi = \pi/2, \theta = \pi/4 \) and \( X_+ = 0 \) yields

\[
q^{vN}(+, x) = -\frac{1}{2}|N_+|^2, \tag{5.40}
\]

so a Lüders bound violation of this more restricted type is possible.

This example is also another example of the interplay between NSIT conditions and LG inequalities and is perhaps even more striking than the example given in Section 5(B), since here both the NSIT condition and the LG inequality that is violated are those for the same dichotomic variable \( \hat{Q} \).

Finally, note that to measure the von Neumann quasi-probability, one way is simply to measure the interference term \( I_{-, 0} \) and add the result to the measured value of \( q(+, x) \). This is possible since any of the three interference terms may be determined experimentally by measuring the degree to which the NSIT conditions such as Eq.(5.21) and Eq.(5.29) are violated, from which the value of any individual interference term may be extracted.

VI. LEGGETT-GARG VIOLATIONS IN THE SIMPLE HARMONIC OSCILLATOR WITH A SINGLE COHERENT STATE

Now we shift our analysis from interference experiments to investigating another common type of experimental setup used in quantum coherence experiments, namely the coherent state of a harmonic oscillator. This work is inspired by a recent discussion by Bose et al [10] which suggests that the “classical-like” coherent state of the harmonic oscillator may still exhibit a significant violation of the LG inequalities. This type of model describes a number of macroscopic oscillator systems that can be realized experimentally, and hence provides a possible path to LG tests on truly macroscopic systems. Bose et al considered the four-time LG inequalities for the coherent state and used numerical methods to calculate the correlators and exhibit a LG violation. Here we take the simpler case of a two-time LG inequality (which will be simpler to measurement experimentally since it only involves one correlator) and determine the correlator analytically.

We suppose that measurements are made which determine whether the particle is in \( x < 0 \) and \( x > 0 \) at each time and the dichotomic variable is taken to be \( \hat{Q} = P_+ - P_- \) where the projectors are \( P_\pm = \theta(\pm \hat{x}) \). We focus on the quasi-probability \( q(-, +) \) which may be
written,

\[ q(-, +) = \text{Re} \langle \psi | e^{iHt} P_+ e^{-iHt} P_- | \psi \rangle \]
\[ = \text{Re} \int_0^\infty dx \, \psi^*(x, t) \langle x | e^{-iHt} P_- | \psi \rangle, \]  

(6.1)

where the initial state is taken to be the gaussian,

\[ \psi(y) = N_s \exp \left( -\frac{y^2}{4\sigma^2} + \frac{ip_0y}{\hbar} \right), \]

(6.3)

where

\[ N_s = \frac{1}{(2\pi \sigma^2)^{1/4}}. \]

(6.4)

The harmonic oscillator propagator is,

\[ \langle x | e^{-iHt} P_- | y \rangle = N_p \exp \left( \frac{im\omega x^2}{2\hbar \sin \omega t} \left[ (x^2 + y^2) \cos \omega t - 2xy \right] \right), \]

(6.5)

where

\[ N_p = \left( \frac{m\omega}{2\pi i\hbar \sin \omega t} \right)^{1/2}. \]

(6.6)

We therefore get

\[ \langle x | e^{-iHt} P_- | \psi \rangle = \int_{-\infty}^0 dy \langle x | e^{-iHt} | y \rangle \psi(y) \]
\[ = \text{Re} \left\{ N_s N_p \int_{-\infty}^0 dy \exp (-ay^2 + iby) \exp \left( \frac{im\omega x^2}{2\hbar \sin \omega t} \cos \omega t \right) \right\} \]

(6.7)

where

\[ a = \left( \frac{m\omega \cos \omega t}{2i\hbar \sin \omega t} + \frac{1}{4\sigma^2} \right), \quad b = \left( \frac{p_0}{\hbar} - \frac{m\omega x}{\hbar \sin \omega t} \right). \]

(6.8)

Evaluating the integral we obtain

\[ \langle x | e^{-iHt} P_- | \psi \rangle = \text{Re} \left\{ N_s N_p \frac{1}{2} \sqrt{\frac{\pi}{a}} e^{-b^2/a} \left( 1 - i\text{erfi} \left( \frac{b}{2\sqrt{a}} \right) \right) \exp \left( \frac{im\omega x^2}{2\hbar \sin \omega t} \cos \omega t \right) \right\}, \]

(6.9)

where \( \text{erfi} \) is the imaginary error function. The quasi-probability is therefore given by

\[ q(-, +) = \text{Re} \left\{ |N_s|^2 |N_p|^2 \frac{\pi}{2|a|} \int_0^\infty dx \, e^{-A z^2(x)} \text{erfi} (iz(x)) \right\}, \]

(6.10)

where we have

\[ z(x) = \frac{b}{2\sqrt{a}} = \frac{1}{2\sqrt{a}} \left( \frac{p_0}{\hbar} - \frac{m\omega x}{\hbar \sin \omega t} \right), \]

\[ A = a \left( \frac{1}{a} + \frac{1}{a^2} \right). \]

(6.11)
Performing a simple change of variables we arrive at a form,
\[
q(-,+)=\text{Re}\left\{ |N_s|^2 |N_p| z(0) \frac{2\pi \hbar \sqrt{a} \sin \omega t}{|a|m\omega} \int_{-\infty}^{z(0)} dz e^{-Az^2} \text{erfi}(iz) \right\}. \tag{6.14}
\]

The remaining integral can be evaluated with the result,
\[
q(-,+)=\frac{1}{4} \left[ 1 + \text{erf} \left( \sqrt{A}z(0) \right) \right] + 4 \text{Re} \left\{ T \left[ \sqrt{2}Az(0), \frac{i}{\sqrt{A}} \right] \right\}. \tag{6.15}
\]

Here, \( T[h,a] \) denotes the Owen T-function \[45\],
\[
T[h,a] = \frac{1}{2\pi} \int_0^a dx \frac{\exp\left(-\frac{1}{2}h^2(1+x^2)\right)}{1+x^2}. \tag{6.16}
\]

The other three components of the quasi-probability are obtained using simple symmetry arguments applied to the above calculation and we find the result,
\[
q(s_1,s_2)=\frac{1}{4} \left[ 1 + s_1 \text{erf} \left( \sqrt{A}z(0) \right) - 4s_1s_2 \text{Re} \left\{ T \left[ \sqrt{2}Az(0), \frac{i}{\sqrt{A}} \right] \right\} \right]. \tag{6.17}
\]

From this we may read off the averages \( \langle \hat{Q}_1 \rangle = 0 \),
\[
\langle \hat{Q}_2 \rangle = \text{erf} \left( \sqrt{A}z(0) \right), \tag{6.18}
\]
and the correlator,
\[
C_{12} = -4 \text{Re} \left\{ T \left[ \sqrt{2}Az(0), \frac{i}{\sqrt{A}} \right] \right\}. \tag{6.19}
\]

The arguments of the error function and T-function have the explicit expressions,
\[
\sqrt{A}z(0) = \frac{\sqrt{2}p_0\sigma}{\hbar} \left( 1 + 4\omega^2 t_s^2 \cot^2(\omega t) \right)^{-\frac{1}{2}}, \tag{6.20}
\]
\[
\frac{i}{\sqrt{A}} = \frac{i}{\sqrt{2}} \left( 1 + 2i\omega t_s \cot(\omega t) \right)^{1/2}. \tag{6.21}
\]

where \( t_s = m\sigma^2/\hbar \) (and is the wave packet spreading timescale for the free particle). For the simple harmonic oscillator coherent state we have \( \sigma^2 = \hbar/(2m\omega) \) and it follows that \( 2\omega t_s = 1 \) and the above expressions simplify to
\[
\sqrt{A}z(0) = \frac{\sqrt{2}p_0\sigma}{\hbar} \left( 1 + \cot^2(\omega t) \right)^{-\frac{1}{2}}, \tag{6.22}
\]
\[
\frac{i}{\sqrt{A}} = \frac{i}{\sqrt{2}} \left( 1 + i \cot(\omega t) \right)^{1/2}. \tag{6.23}
\]
FIG. 8: The quasi-probability $q(−, +)$ for the simple harmonic oscillator as a function of $\omega t$ for the case $p' = p_0\sigma/\hbar = −1$. It shows a region of negativity with lowest value approximately $−0.011$.

The free particle case is obtained by taking the limit $\omega \to 0$ in Eqs. (6.20), (6.21), and we have

$$\sqrt{A}z(0) = \frac{\sqrt{2p_0\sigma}}{\hbar} \left(1 + \frac{1}{\tau^2}\right)^{-\frac{1}{2}},$$  

(6.24)

$$\frac{i}{\sqrt{A}} = \frac{i}{\sqrt{2}} \left(1 + \frac{i}{\tau}\right)^{1/2},$$  

(6.25)

where $\tau = t/(2t_0)$. This therefore has exactly the same form as the simple harmonic oscillator case with $\tan(\omega t)$ replaced by $\tau$, and therefore the plots of each are identical with the appropriate parameterization.

A plot of the quasi-probability $q(−, +)$ is shown in Figure 8. It shows negativity (LG violation) for a range of $\tau$, although the negativity is quite a long way from the maximum negativity in the quasi-probability of $−0.125$. The other three quasi-probabilities exhibit no negativity and also show the expected quasi-classical behaviour.

It is also of interest to see the form of the correlator Eq. (6.19) and this is shown in Figure 9 for fixed momentum. It becomes close to a pair of straight lines for large $p$, which is what one would expect on classical grounds. A natural situation to explore using this correlator
FIG. 9: The correlator $C_{12}$ for the simple harmonic oscillator as a function of $\omega t$, with $p' = -1$.

would be a set of three-time or four-time LG inequalities (noting that four-time inequalities were explored in Ref. [10]). However, we have found that the initial state used here is too restrictive to get any interesting results. The issue is that the above analytic calculation leading to the correlator Eq. (6.19) is only relevant to situations in which the system is in a state of the form Eq. (6.3) at the beginning or end of each time interval. Future work will address this.

We make some final comments to contrast the LG violations for the simple harmonic oscillator in a gaussian state with the LG violations in interference experiments. The quasi-probability $q(s_1, s_2)$ of the form Eq. (2.5) may be conveniently written using the Wigner representation [46] as

$$q(s_1, s_2) = 2\pi\hbar \int dX dp \ W_{s_1 s_2}(X, p)W_\rho(X, p), \hspace{1cm} \text{(6.26)}$$

as discussed in Ref. [12]. Here, $W_\rho(X, p)$ is the Wigner transform of the initial state $\rho$,

$$W_\rho(X, p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} d\xi \exp \left( -\frac{i}{\hbar} p\xi \right) \rho(X + \frac{1}{2}\xi, X - \frac{1}{2}\xi), \hspace{1cm} \text{(6.27)}$$

and $W_{s_1 s_2}(X, p)$ is the same transform of the operator,

$$A_{s_1 s_2} = \frac{1}{2} \left( P_{s_1}(t_1)P_{s_2}(t_2) + P_{s_2}(t_2)P_{s_1}(t_1) \right). \hspace{1cm} \text{(6.28)}$$
The quantities $W_{s_1 s_2}(X,p)$ and $W_p(X,p)$ tend to be largely positive in phase space, with occasional oscillations to negative values. There are therefore two distinct ways in which $q(s_1, s_2)$ may become negative and we get a two-time LG violation – it can come predominantly from the state or predominantly from the operator $A_{s_1 s_2}$.

For the superposition states considered in the interference experiments the Wigner functions are negative and this is the primary source of the LG violation (noting also that the essentially semi-classical approximations used will probably render $W_{s_1 s_2}(X,p)$ non-negative). For the gaussian state by contrast, the Wigner function is always non-negative, hence for the harmonic oscillator case considered in this section, the LG violation comes from the negativity of $W_{s_1 s_2}(X,p)$ (whose explicit form is given in Ref. [12] for the free particle case). Hence the LG violations in each case have quite different origins. Note also that in the latter case, the negativity of $W_{s_1 s_2}(X,p)$ is related to the sharpness of the projectors. In a realistic experimental situation the measurements will correspond to smoothed out projectors and one would expect the negativity of $W_{s_1 s_2}(X,p)$ and the subsequent LG violation to be lessened, so a more detailed analysis is required to estimate how smooth the projectors can be whilst still maintaining a LG violation. This will be explored in more detail elsewhere.

VII. SUMMARY

We have explored LG tests for macrorealism in a number of systems described by continuous variables: the double-slit experiment, the triple-slit experiment and the free particle and simple harmonic oscillator in a gaussian state. These systems are of particular interest in the drive to develop LG tests for progressively larger systems with some claim towards being macroscopic.

In the double-slit case, we found that LG violations are essentially always accompanied by destructive interference, although not conversely in general, except for special parameter values. Hence there is a relationship between two different notions of quantumness. However, the fact that destructive interference does not always imply LG violation means that there are situations in which one can in fact assign probabilities to the paths in an interferometer, using an indirect procedure, even when destructive interference is present. I.e. there is in some circumstances an underlying classical model of a situation commonly thought of as “quantum”.

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We also examined the related question of what happens if measurements of varying strength are used to determine which slit the particle passes through and how the measurement strength affects the interference pattern, using the convenient formalism of ambiguous measurements. Our results are very much in line with earlier work in this area which indicates the interference is still present even in the face of a high degree of certainty as to which slit the particle went through. This approach is not a LG test but the path probabilities obtained coincide with those obtained from the LG analysis in the limit of weak measurement.

The triple-slit experiment revealed a rather different and more fluid relationship between destructive interference and LG violation, due to the fact that it involves three independent interference terms, rather than just the one present in the double-slit case. In fact we found that LG violations could arise without any destructive interference being present. More specifically, we showed that it is possible to have a NSIT condition satisfied (which implied zero interference at the screen) but at the same time have LG violations. We also showed that the triple-slit experiment can exhibit a simplified version of the Lüders bound violation. These two features illustrate general properties of many-valued systems outlined in Ref. [6].

In these interference experiments, LG violations arose due to the presence of superposition states in position. We therefore explored a very different situation involving the free particle and simple harmonic oscillator in a single gaussian state. Despite the initial state having non-negative Wigner function, LG violations are still possible. This provides a simpler and analytically tractable example of the the LG violations discussed in Ref. [10]. A future paper will explore LG tests for a variety of experimentally accessible states of the simple harmonic oscillator in considerably more detail [47].

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