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## A Review of the Leggett-Garg Framework and Violations of Macrorealism.

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#### Abstract

The notion of macrorealism and associated assumptions was first proposed by Leggett and Garg in 1985 in the hope of testing quantum behaviour against classical intuition. Mainly, there are three assumptions that a macrorealistic system should obey: (i) physical quantities of a system should have definite values at all times (macrorealism per se), (ii) it is possible to measure these quantities without disturbing the future evolution of the system (non-invasive measurability), and (iii) future measurements cannot affect the system in the past (induction). Similarly to Bell's case, Leggett and Garg derived a set of inequalities consisting of time correlation functions, which a macrorealistic system should satisfy. In this review, we thoroughly discuss the formulation and the validity of the Leggett-Garg framework and possible generalizations of the framework in testing larger systems. We also include the discussion on how the Leggett-Garg inequalities can be combined to form a set of necessary and sufficient conditions for macrorealism, a consideration that has been lacking in many previous experiments, and comparisons between different versions of macrorealism. We also present a quantum-mechanical formulation of the Leggett-Garg inequalities to highlight what the LG framework actually tests. We have shown that LGIs are only satisfied when the interference caused by measurements is sufficiently small, and violations can be found across a variety of quantum systems. Since measurements are inherently invasive on a quantum system, different experiment set-ups would require separate justifications for non-invasiveness and they do not hold in the general case. As a result, a clumsiness loophole always exists, where a macrorealist would argue that violation is caused by measurements being invasive after all, and macrorealism per se cannot be refuted. There are various proposals to narrow or even close this loophole, but this proves to be challenging and needs to be carefully assessed in future experiments.

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# Chapter 1

## Introduction

In recent years, means to probe the behaviour of quantum systems and certify quantum coherence within have become increasingly in demand, and the ability to do so is critical, especially in the blooming fields of quantum biology and quantum information processing. The difficulty being any interaction with the system through measurements on a quantum system will collapse the wavefunction, hindering us from assessing the existence of genuine quantum behaviour. This feature of quantum mechanics is in stark contrast to classical objects from our intuition.

A novel approach has been proposed by Leggett and Garg in their 1985 paper[1], initially to address the question: "is the (quantum) flux there when nobody looks". Leggett and Garg have proposed a set of criteria that a classical system would obey, and the conjunction of these criteria is known as macrorealism. Based on these assumptions, a set of inequalities, known as the Leggett-Garg inequalities, are derived, for which a macrorealistic system would satisfy. As discussed in this review, these inequalities not only address the more philosophical questions, such as the compatibility between quantum mechanics and physical reality, but also serve as a coherence witness in certifying the level of "quantumness" present in any given system.

The Leggett-Garg inequalities, constructed from time correlation functions, take different forms depending on the particular system we are trying to test, and the set of necessary and sufficient conditions varies depending on the measurement scheme. They can be viewed as a generalization to the Bell/CHSH inequalities, sometimes referred to as the temporal version of Bell inequalities, but with a few caveats. Extra considerations, as we will discuss later, must be taken in order to recreate the success of Bell inequalities in disputing local realism.

This review will structure as follows. In Chapter 2, we review the derivation of the Leggett-Garg inequalities as they were initially proposed, and together with a discussion on the types of measurements that can be used in a Leggett-Garg test, we aim to present the original LG framework, albeit incomplete, on testing quantum systems. In chapter 3, we focus more on the notion of macrorealism, and discuss how the LGIs can be combined to obtain a set of necessary and sufficient conditions for macrorealism by utilizing Fine's theorem, thereby completing the LG framework.

We will also show how the complete LG framework can be readily extended to test larger systems and note possible versions of macrorealism and comparisons between them. We close by discussing a few recently performed experiments and an overview of the LG framework in Chapter 4.

## Chapter 2

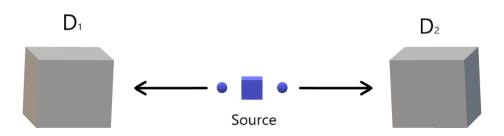
## Laggett-Garg Framework

### 2.1 Motivations

Object permanence, the understanding that things continue to exist when they are not seen, is developed by infants at as early as eight to nine months of age. The idea that the properties of a system continue to behave in the same way when they are not being observed as they do when they are being observed is buried deeply in everyone's intuition. The notion that the existence of reality is independent of observation is known as *realism*, one of the trivial assumptions of classical physics. This is rarely challenged until the development of quantum mechanics.

Realism implies that the variables describing a system must possess definite values at all times, independent of observations, which then implies that an underlying probability distribution describing these variables must exist. On the other hand, in the Copenhagen interpretation of quantum mechanics, it is believed that quantum systems exist in superpositions of states (described by wavefunctions) in between observations (or measurements); therefore, reality will not be in a definite state until it is observed. Furthermore, quantum theory assigns probabilities only to sets of commuting variables, and an underlying probability distribution for all the variables may not exist. As we will also discuss in Chapter 3, testing realism, at its core, is all about probing the existence of underlying joint probability distribution.

This leads to the famous Einstein-Podolsky-Rosen (EPR) paradox[2]. Consider a pair of entangled spin  $\frac{1}{2}$  particles which have spin in the same direction and are spatially separated by some arbitrary distance. The spin of the particles are measured simultaneously along some axis by two detectors  $D_1$  and  $D_2$  with outcomes  $(s_1, s_2) \in \{\pm 1\}$  such that  $s_1 = s_2$ . It is argued that if the entangled system is not in a definite state before the measurements, then there must be instantaneous communication between the two particles when they are being measured to always produce the same outcome. Einstein argued that this instantaneous communication must violate *locality*, which is the idea that the influence of an event at one point can not travel faster than the speed of light, therefore, the measurement outcomes must have been predetermined by local hidden variables which are only revealed during



**Figure 2.1:** A simple illustration of the experimental set-up in the EPR paradox and Bell experiment. The source generates two entangled particles in a way that their spins will always point in the same direction. The particles then move in the opposite direction towards the two detectors,  $D_1$  and  $D_2$ , which are spacelike separated. Both detectors will measure the incoming particle's spin along a certain direction, and the outcomes will be  $\pm 1$ .

the measurements. Based on Einstein's assumptions regarding locality, the paper then claims that quantum mechanics is, in fact, "incomplete", and that the local hidden variables are there to protect the "element of reality". This is known as the local hidden variable theory, an alternative theory to the Copenhagen interpretation to protect (local) realism.

Both theories predict the same measurement outcomes in the EPR paradox, therefore, these two views of reality remain at a standstill. However, in 1964, John Bell demonstrated that they could be distinguished with a more refined measurement scheme than the one described in the EPR paradox. In this set-up, both detectors  $D_1, D_2$  are able to measure the spin of the particle along three co-planar axis,  $\alpha, \beta, \gamma$ , which are separated by 120°. During each measurement, each detector will choose a random axis to produce an outcome of either +1 or -1. As we will show below, there is a discrepancy between the probability of obtaining the same outcome on  $D_1$ and  $D_2$ , e.g.  $p(s_1 = s_2)$ , as predicted by these two theories.

According to the local hidden variable theory, the outcome is determined when the particles are generated. Then, there are only  $2^3 = 8$  possible definite states the particles could be in, they are (+1, +1, +1), (+1, +1, -1), (+1, -1, +1), (+1, -1, -1), (-1, +1, +1), (-1, +1, -1), (-1, -1, +1) and (-1, -1, -1), where each of the three numbers corresponds to the measurement outcome in axis  $\alpha, \beta, \gamma$  respectively. Out of the eight possibilities, there are two cases, namely (+1, +1, +1) and (-1, -1, -1), which will guarantee  $p(s_1 = s_2) = 1$  regardless which axis each detector chooses. In the remaining six cases, it can be shown that  $p(s_1 = s_2) = \frac{5}{9}$ , see **Table 2.1** for an example.

Therefore, the probability of both detectors giving the same outcome according to the local hidden variable theory is:

$$p(s_1 = s_2) = \left(\frac{2}{8} \times 1\right) + \left(\frac{6}{8} \times \frac{5}{9}\right) = \frac{2}{3} \approx 0.667.$$
 (2.1)

Now we calculate the same probability according to the Copenhagen interpretation. Without affecting the conclusion of the experiment, we assume that  $D_1$  per-

	( $D_1$ ) Axis $\alpha$	( $D_1$ ) Axis $\beta$	( $D_1$ ) Axis $\gamma$
( $D_2$ ) Axis $\alpha$	Same	Different	Same
( $D_2$ ) Axis $\beta$	Different	Same	Different
( $D_2$ ) Axis $\gamma$	Same	Different	Same

**Table 2.1:** This is a list comparing the measurement outcomes from two detectors  $D_1$  and  $D_2$  in a Bell experiment for the initial state (+1, -1, +1) according to local hidden variable theory. Each detector will choose one random axis to measure along, and it shows that, out of the nine possible pairs of the chosen axis, five pairs will return the same result. Given that the axis is chosen on random, there is a  $\frac{5}{9}$  probability of both detectors measuring the same result. The same probability hold for all the initial states where the spins along the three directions have only two of the same value.

forms the measurement first at  $t = t_0$ , and then  $D_2$  performs the measurement at  $t = t_0 + \delta$ , with the distance  $d = \delta \times c$  much smaller than the spatial separation between the two particles, e.g. locality will still be violated. In this case, as soon as  $D_1$  makes the measurement, the wavefunction will collapse, and the particles will be in a definite state. Regardless of the chosen axis of detector  $D_1$ , detector  $D_2$  would have chosen the same axis with a probability of  $p(same axis) = \frac{1}{3}$ , which will then yield the probability  $p(s_1 = s_2 | same axis) = 1$ , since the two particles are entangled. If  $D_1$  and  $D_2$  has chosen different axis for their measurements, with a probability of  $p(different axis) = \frac{2}{3}$ , then probability  $p(s_1 = s_2 | different axis)$  is given by the projection of spin measured by  $D_1$  onto the chosen axis of  $D_2$ , and quantum mechanics tells us that  $p(s_1 = s_2 | different axis) = cos \left(\frac{120^\circ}{2}\right)^2 = \frac{1}{4}$ . Thus, the probability of both detectors giving the same outcome according to the Copenhagen interpretation is equal to:

$$p(s_1 = s_2) = \left(\frac{1}{3} \times 1\right) + \left(\frac{2}{3} \times \frac{1}{4}\right) = \frac{15}{36} \approx 0.416.$$
 (2.2)

This discrepancy between the predicted value of the probability allows us to test the existence of local realism experimentally.

A set of inequalities can also be derived from the experimental set-up above to serve as a more practical test for local realism. We now denote the measurement outcomes as  $s_X^i$ , where  $i \in \{1, 2\}$  denotes the corresponding detectors  $D_i$  and  $X \in \{\alpha, \beta, \gamma\}$  denotes the axis chosen by detector  $D_i$ .

From the eight possibilities according to the local hidden variable theory listed above, it is straight forward to see that the values of  $s_X^1$  have at least 2 of the same value, therefore, the union of the events  $\{s_{\alpha}^1 = s_{\beta}^1\}$ ,  $\{s_{\beta}^1 = s_{\gamma}^1\}$  and  $\{s_{\alpha}^1 = s_{\gamma}^1\}$  must equal to the entire sample space. Therefore the following equation must be true (see also Table 2.2):

$$p(s_{\alpha}^{1} = s_{\beta}^{1}) + p(s_{\beta}^{1} = s_{\gamma}^{1}) + p(s_{\alpha}^{1} = s_{\gamma}^{1}) \ge 1.$$
(2.3)

We have been considering two entangled particles which have their spin perfectly correlated, and this implies  $s_{\alpha}^1 = s_{\alpha}^2$ , when substituted into inequality (2.3), gives

$(s^1_lpha, s^1_eta, s^1_\gamma)$	$p(s^1_\alpha = s^1_\beta)$	$+p(s^1_\beta=s^1_\gamma)$	$+p(s^1_\alpha=s^1_\gamma)$	=
(+1,+1,+1)	1	1	1	3
(+1,+1,-1)	1	0	0	1
(+1, -1, +1)	0	0	1	1
(+1, -1, -1)	0	1	0	1
(-1,+1,+1)	0	1	0	1
(-1, +1, -1)	0	0	1	1
(-1, -1, +1)	1	0	0	1
(-1, -1, -1)	1	1	1	3

**Table 2.2:** This is a list of the probabilities that measurements of spin along two of the three possible directions will have the same value. All of the  $2^3 = 8$  possible initial states in a Bell experiment according to the local hidden variable theory are considered here. The last column on the right is the sum of the probabilities, and it is easy to see that the sums are either 1 or 3.

inequalities of the form:

$$p(s_{\alpha}^{1} = s_{\beta}^{2}) + p(s_{\beta}^{1} = s_{\gamma}^{2}) + p(s_{\alpha}^{1} = s_{\gamma}^{2}) \ge 1.$$
(2.4)

These inequalities are known as the Bell inequalities. If the system we are considering is perfectly anti-correlated, e.g.  $s_{\beta}^1 = -s_{\beta}^2$ , we can find the new set of Bell inequalities by replacing the equal signs with not equal signs within the arguments of the probabilities.

It is also worth noting that the derivation of the Bell inequalities given above is solely based on a complete list of permutations of 3 dichotomic random variables, which take on values of  $\pm 1$ . The data set we are considering here could have any reasonable context, they could be the results of three fair coin tosses or they can be devoid of any statistical meaning. Either way, inequality (2.3) appears trivially satisfied, as shown in **Table 2.2**. However, the Bell inequalities (2.4) are violated by quantum mechanics. As calculated above,  $p(s_X^i = s_Y^j) = \frac{1}{4}$  for  $i \neq j$  and  $X \neq Y$ , this results in the left hand side of the Bell inequalities (2.4) to add up to  $\frac{3}{4}$  which means the inequality is violated. This is a significant result which proves that quantum mechanics is incompatible with the notion of local realism described by Einstein.

There is also a generalisation of the Bell inequalities developed by John Clauser, Michael Horne, Abner Shimony and Richard Holt (CHSH), which applies to situations where the assumption of perfect correlations or anti-correlations no longer holds. For the derivation of CHSH inequalities, we consider the following set-up and notation. Similar to the previous set-up, we have a spatially separated pair of entangled particles whose spins are highly-correlated. Spin on the first particle are measured along the axis **a** or **a'**, we denote the measurement outcomes as  $s_1$  and  $s_2$  respectively with values of  $\pm 1$ . Similarly, the second particle's spin is measured along axis **b** and **b'** with outcomes  $s_3$  and  $s_4$ . Following the idea of local hidden variable theory, there are two cases: either  $s_1 + s_2 = 0$  and  $s_1 - s_2 = \pm 2$ , or  $s_1 - s_2 = 0$  and  $s_1 + s_2 = \pm 2$ . We can define a function S as :

$$S \equiv (s_1 + s_2)s_3 + (s_1 - s_2)s_4 = s_1s_3 + s_2s_3 + s_1s_4 - s_2s_4 = \pm 2,$$
(2.5)

such that the following holds,

$$|S| = |(s_1 + s_2)s_3| + |(s_1 - s_2)s_4| = |s_1s_3 + s_2s_3 + s_1s_4 - s_2s_4| \le 2.$$
(2.6)

Assuming an underlying probability distribution  $p(s_1, s_2, s_3, s_4)$  exists, then we can immediately obtain the following inequality from inequality (2.6):

$$|S| \le \sum_{s_1, s_2, s_3, s_4} |s_1 s_3 + s_2 s_3 + s_1 s_4 - s_2 s_4 | p(s_1, s_2, s_3, s_4) \le |C_{13} + C_{23} + C_{14} - C_{24}| \le 2,$$
(2.7)

where we have introduced the correlation functions  $C_{ij}$  defined as,

$$C_{ij} = \sum_{s_1, s_2, s_3, s_4} s_i s_j p(s_1, s_2, s_3, s_4).$$
(2.8)

Inequality (2.7) is one of the CHSH inequalities, and there are three more which can be obtained by permuting the minus sign to three other possible locations. Just like the Bell inequalities, examples of violations of the CHSH inequalities by quantum systems can be readily found; see ref [3; 4; 5]. Arthur Fine later published a paper[6] and proved that Bell and CHSH inequalities are, in fact, necessary and sufficient conditions for local realism. This result is known as *Fine's theorem*, which is discussed in detail in Chapter 3. Since their invention, experimental violations of Bell and CHSH inequalities have been tested on a variety of quantum systems, together, these results suggest quantum mechanics indeed violate Einstein's notion of local realism, even though the implications of the violation is still heavily debated[7].

To be explicit, Einstein, Podolsky and Rosen, in their original paper, gave a clear definition of their notion of realism, commonly referred to as EPR *Criterion of Reality*[2].

If, without in any way disturbing a system, we can predict with certainty (i.e., with probability equal to unity) the value of a physical quantity, then there exists an element of reality corresponding to that quantity.

In quantum mechanics, a quantity can only be determined without disturbing the system only if the quantum state is an eigenstate of said quantity, and the value will be the corresponding eigenvalue of that state. However, for a pair of incompatible quantities, e.g., position and momentum, a quantum state, which is an eigenstate of both quantities simultaneously, is simply not permitted. In other words, joint probabilities for position and momentum are ill-defined in any given quantum state, according to quantum mechanics. This is why Bell and CHSH inequalities can be violated since the existence of such joint probabilities is a key assumption in both derivations. Another important issue to address is the violation of locality. The

notion of locality is motivated by Einstein's special theory of relativity, however, a violation of locality does not imply a violation of causality. The entangled particles with their spins correlated, as mentioned above, cannot be used to send information between the locations of the detectors, which are space-like separated. Any exchange of information would still require a classical channel, hence, causality is not violated. In this context, quantum mechanics is often referred to as *non-local* since the entangled states with non-local (not predetermined) correlation are allowed. It is in this way, we conclude that quantum mechanics violate local realism.

Violations of Bell and CHSH inequalities do not prove the Copenhagen interpretation of quantum mechanics, but instead, they allowed us to rule out the local hidden variable theories. The discussions and conclusions sparked other theories, such as the de Broglie-Bohm theory of quantum mechanics[8] and the many-worlds interpretation of quantum mechanics, also known as the Everett interpretation[9]. Ultimately, the EPR paradox and Bell/CHSH tests deepened the understanding of the underlying nature of quantum mechanics and enticed further developments in this field, and the implications of their work on the foundations of quantum theory are still being debated to date.

### 2.2 Assumptions of Macrorealism

All of our discussions so far are in fact part of a bigger question: how and when do classical properties emerge from quantum mechanics? In exploring where the classical limit lies, we inevitably wonder if *macroscopic coherence* is achievable, a type of phenomenon that macroscopic systems composed of very many atoms exhibiting quantum behaviour and existing in a superposition of macroscopically distinct state. If it is possible to achieve this, how would we then test the "quantumness" in a system and prove the existence of said phenomenon? This problem is addressed in a 1985 paper by Leggett and Garg[1].

Leggett and Garg started off by proposing a set of assumptions to their intuition of the macroscopic world, and they are as follows[1]:

- 1. Macroscopic realism per se (MRps): a macroscopic system with two or more macroscopically distinct states available to it will at all times be in one or the other of these states.
- 2. Noninvasive measurability (NIM): it is possible, in principle, to determine the state of the system with arbitrarily small perturbation on its subsequent dynamics.

In more-recent papers[10], Leggett and Garg added the third assumption for completeness, but it is rarely contested:

3. Induction: the outcome of a measurement on the system cannot be affected by what will or will not be measured on it later.

The conjunction of these assumptions is coined the name macrorealism (MR).

A fitting example would be that of the well-known Schrödinger's cat. According to quantum mechanics, the cat, exhibiting macroscopic coherence, must be simultaneously dead and alive before the wavefunction collapses as we open the box. Under a theory which admits the assumptions of MR, however, the cat must be either dead *or* alive at any given time, and it can be measured in a way that neither affect nor affected by the final fate of the poor cat[11]. Therefore, this notion of macrorealism aligns with our intuition of physical reality but strongly contradicts the predictions of quantum mechanics.

Note that the reason that the first assumption is commonly referred to as MRps is to distinguish it with MR, which often thought of as "macrorealism in the broader sense". There are many criticisms and debates regarding these assumptions' exact interpretations and validity, especially the first two, MRps and NIM. We will temporarily ignore these issues until Chapters 3 and follow the arguments of the original paper to derive a set of inequalities similar to those of Bell and CHSH. The main takeaway from these assumptions is that MR, as Leggett and Garg initially presented them, aligns with the notion of realism we have been discussing so far, that the physical quantities corresponding to a macrorealistic system should be deterministic at all times, independent of measurements.

### 2.3 Derivation of LGIs

Consider a time-evolving system where we measure a single dichotomic variable, Q(t), at times,  $t_i$ , and we will assume that  $t_1 < t_2 < t_3$ .... For simplicity, we will denote  $Q(t_i)$  as  $Q_i$ . And, to be consistent with our previous notation, the outcome of the measurements of  $Q_i$  will be denoted as  $s_i$ , similar to the Bell case, can be either +1 or -1.

Then it immediately follows from the conclusion of the last subsection, for a macrorealistic system, joint probability distributions exists, e.g.,  $p(s_1, s_2)$ ,  $p(s_1, s_2, s_3)$ , and also are consistent with one another, e.g.,

$$\sum_{s_1=\pm 1} p(s_1, s_2, s_3) = p(s_2, s_3).$$
(2.9)

We can then also define averages  $\langle Q_i \rangle$  and correlation functions,  $C_{ij}$ ,

$$C_{ij} = \langle Q_i Q_j \rangle = \sum_{s_i, s_j = \pm 1} s_i s_j p_{ij}(s_i, s_j).$$
(2.10)

Consider now we perform three separate experiments with the same system, where we measure at  $t = t_1, t_2, t = t_2, t_3$  and  $t = t_1, t_3$  only in each experiment to obtain  $C_{12}$ ,  $C_{23}$  and  $C_{13}$ . Then for a macrorealistic system, these correlation functions can be shown to obey the following inequalities:

$$1 + C_{12} + C_{23} + C_{13} \ge 0 \tag{2.11}$$

$$1 - C_{12} - C_{23} + C_{13} \ge 0 \tag{2.12}$$

$$1 - C_{12} + C_{23} - C_{13} \ge 0 \tag{2.13}$$

$$1 + C_{12} - C_{23} - C_{13} \ge 0 \tag{2.14}$$

These are known as the three-time Leggett-Garg inequalities (LGIs, also abbreviated as LG3s, for reasons to become apparent later), and they have the same mathematical structure as the Bell inequalities.

Following the arguments of Leggett in his 2008 paper[10], we can derive this set of inequalities as follows. Under the assumption of MRps and NIM,  $Q_i$ , for  $i \in \{1, 2, 3\}$ , will always take on a definite value of  $\pm 1$ , irrespective of whether  $Q_i$  is measured or not, provided that the first measurement of every pair in each experiment are measured in a non-invasive way. Also, the value of  $s_i$  is unaffected by what will or will not be measured at a later time, according to the assumption of induction. Thus, we can conclude that for each run, quantities  $Q_iQ_j$  exist, with  $Q_i$  having the same value for any  $t_j$ .

Provided that quantities  $Q_i$  and  $Q_iQ_j$  are well-defined for all  $i, j \in \{1, 2, 3\}$  and  $i \neq j$ , we can then define functions of the form below:

$$Q_{sum} = Q_1 Q_2 + Q_2 Q_3 + Q_1 Q_3, (2.15)$$

$s_1$	$s_2$	$s_3$	$+Q_1Q_2$	$+Q_{2}Q_{3}$	$+Q_{1}Q_{3}$	$= Q_{sum}$
+1	+1	+1	+1	+1	+1	3
+1	+1	-1	+1	-1	-1	-1
+1	-1	+1	-1	-1	+1	-1
+1	-1	-1	-1	+1	-1	-1
-1	+1	+1	-1	+1	-1	-1
-1	+1	-1	-1	-1	+1	-1
-1	-1	+1	+1	-1	-1	-1
-1	-1	-1	+1	+1	+1	3

**Table 2.3:** Values of  $Q_{sum}$  for possible combinations of values of  $s_i$ . It is straight forward to confirm that they are between 3 and -1.

$s_1$	$s_2$	$s_3$	$-Q_1Q_2$	$-Q_2Q_3$	$+Q_{1}Q_{3}$	$=Q_{sum}^{\prime}$
+1	+1	+1	-1	-1	+1	-1
+1	+1	-1	-1	+1	-1	-1
+1	-1	+1	+1	+1	+1	3
+1	-1	-1	+1	-1	-1	-1
-1	+1	+1	+1	-1	-1	-1
-1	+1	-1	+1	+1	+1	3
-1	-1	+1	-1	+1	-1	-1
-1	-1	-1	-1	-1	+1	-1

**Table 2.4:** Values of  $Q'_{sum}$  for possible combinations of values of  $s_i$ . If we consider other functions of the same form as  $Q'_{sum}$ , found by moving the plus sign to other two possible positions, we will find essentially the same table but with the rows on the right half of the table swapped places. In all cases, a lower bound of -1 is always trivially satisfied.

or,

$$Q'_{sum} = -Q_1 Q_2 - Q_2 Q_3 + Q_1 Q_3.$$
(2.16)

These functions will have different values depending on values of  $Q_i$ . By considering the possible values of  $Q_{sum}$  and  $Q'_{sum}$ , by trivial algebra, we find that (see **Table 2.3** and **Table 2.4**):

$$3 \ge Q_{sum} \ge -1,\tag{2.17}$$

the same is also true for  $Q'_{sum}$ , as well as the two more functions found by moving the plus sign to other possible positions.

Here we note that, even if we have prepared all of our experiments in the same way, that they are all in the exact same initial state at  $t = t_0$ , we may still get a statistical spread of values  $\pm 1$ . For it is possible that there are underlying variables at play which are not fixed by our preparation procedure[12]. Therefore, the essential and experimentally accessible quantities will be the expectation values of the form  $\langle Q_i \rangle$  and  $\langle Q_i Q_j \rangle$ . Then by considering the expected value of the functions  $Q_{sum}$  and  $Q'_{sum}$ , we find the inequalities of the form:

$$\langle Q_{sum} \rangle_{all} \equiv \langle Q_1 Q_2 \rangle_{all} + \langle Q_2 Q_3 \rangle_{all} + \langle Q_1 Q_3 \rangle_{all} \ge -1, \tag{2.18}$$

where the subscripts,  $\langle ... \rangle_{all}$ , can have two equivalent meanings. They could indicate that these values correspond to the average taken over *all* runs of the experiment, i.e., we are merging results from all three experiments. Or equivalently, they could be thought of as indicating a single experiment, where we measure at *all* three times. Either way, we disregard which measurements took place in each experiment and consider all data equally. Note that we have left out the upper bound in inequality (2.18), it is irrelevant in experimental studies since only the lower bound is found violated by quantum mechanics[11].

Inequality (2.18) looks very similar to the LGI (2.11) already. However, there is one crucial difference. When considering the case where measurements are performed at all three times in a single experiment, it is easy to see that inequality (2.18) must always hold, even in quantum mechanics. Since regardless of the fact whether the quantity Q(t) has deterministic values or not prior to a measurement, the measurement outcomes must be definitive, and there exist joint probabilities of outcomes for a sequence of (commuting) performed measurements.

To get to the LGIs, we need to invoke the assumption of NIM. If both measurement at times,  $t = t_1$  and  $t = t_2$ , are performed in a non-invasive way, such that future evolution of the system is not at all affected the first two measurements, then the measurement at time  $t = t_3$  should have the same outcome, regardless of measurements at  $t = t_1$  or  $t = t_2$  are actually performed. Therefore, under the assumption of NIM, we have that:

$$C_{ij} \equiv \langle Q_i Q_j \rangle_{i,j} = \langle Q_i, Q_j \rangle_{all}, \qquad (2.19)$$

where the subscript  $\langle ... \rangle_{i,j}$  indicate that measurements are taken twice at  $t = t_i$  and  $t = t_j$  only. Here we stress that the commutation functions,  $C_{ij}$ , that appear in LGIs are valid when measurements are taken at labelled times *only*.

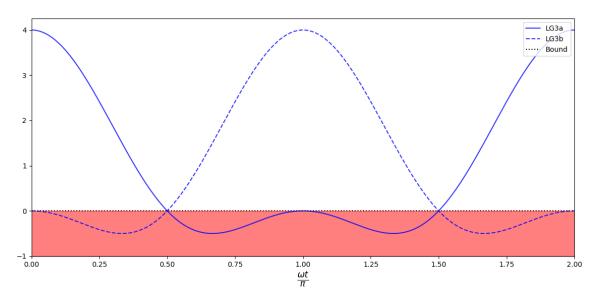
By substituting equation (2.19) into inequality (2.18) and similar inequalities obtained by considering  $Q'_{sum}$ , we arrive at the usual three-time LGIs (inequalities (2.11)-(2.14)). Unlike inequality (2.18), which states a trivial algebraic feature that the measured outcomes of  $Q_i$  from a single experiment must satisfy, LGIs relate the results from three distinct experiments in a highly non-trivial way.

Violation of LG3s can be found if we consider the following set-up: a spin- $\frac{1}{2}$  particle evolving under a Hamiltonian  $\hat{H} = \frac{1}{2}\omega\hat{\sigma_x}$ , and the spin is measured along the z-direction,  $\hat{Q} = \hat{\sigma_z}$ . The quantum analogue of the classical correlation function,  $C_{ij}$ , according to Fritz[13], can be found to be half the expectation value of the anti-commutator of the observables when using projective measurements (see discussions later),

$$C_{ij} = \frac{1}{2} \left\langle \left\{ \hat{Q}_i, \hat{Q}_j \right\} \right\rangle, \qquad (2.20)$$

In this case, it can be shown that the correlation functions take the simplified form[11]:

$$C_{ij} = \frac{1}{2} \left\langle \hat{Q}_i \hat{Q}_j + \hat{Q}_j \hat{Q}_i \right\rangle = \cos(\omega(t_j - t_i)).$$
(2.21)



**Figure 2.2:** A plot of the values of the left-hand side of the LG3s, for a simple qubit-like system, with the region below the bound of zero coloured red, indicating a violation. The four LG3s are reduced to two non-trivial ones, namely LG3a (2.22) and LG3b (2.23). As can be seen in the plot, LG3a is violated for  $\frac{\pi}{2} < \omega t < \frac{3\pi}{2}$  and LG3b is violated in regions  $\omega t < \frac{\pi}{2}$  and  $\omega t > \frac{3\pi}{2}$ . Interestingly, there are cases where for certain value of  $\omega t$ , namely  $\omega t = \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ , the LG3s are not violated.

For simplicity, we consider the case  $t_2-t_1 = t_3-t_2 = t$ . Then the LGIs (2.11)-(2.14) simplify to:

$$(LG3a)1 + 2\cos(\omega t) + \cos(2\omega t) \ge 0,$$
 (2.22)

$$(LG3b)1 - 2cos(\omega t) + cos(2\omega t) \ge 0,$$
 (2.23)

$$1 - \cos(2\omega t) \ge 0. \tag{2.24}$$

Where we note inequalities (2.13) and (2.14) both simplify to the same inequality (2.24) and are always trivially satisfied. By plotting the inequalities (2.22) and (2.23) as a function of  $\omega t$ , we find that LGIs are violated by this system at all times, except for specific discrete values of  $\omega t$ , see **Figure 2.2**.

We have now successfully found a case where the LGIs are violated. The exact implications of violations of LGIs, however, are still heavily debated; see later chapters for more discussion. Ever since the first example of violation given in the original paper by Leggett and Garg[1], violations of the LGIs are found experimentally on a variety of quantum systems, see Refs [14; 11; 15; 16].

### 2.4 Alternative Derivation of LG3s

In this subsection, we consider an alternative derivation of the LG3s, a perhaps more explicit way of arriving at the same set of conditions.

Again, following the assumption of MRps, the variable Q(t) will take definite values at all times. We can then define the two-time probabilities as:

$$p_{ij}(s_i, s_j) = \sum_{s_k = \pm 1} p_{ij}(s_1, s_2, s_3),$$
(2.25)

where the subscripts  $p_{ij}(...)$ , again, signify that the probability is obtained by performing measurements at times  $t = t_i$  and  $t = t_j$  only.

Then, under the assumptions of NIM and induction, we can expect that the probability of the measurement outcomes should be independent of whether earlier or later measurements are made. This leads to the following expression:

$$p_{12}(s_1, s_2, s_3) = p_{13}(s_1, s_2, s_3) = p_{23}(s_1, s_2, s_3) \equiv p(s_1, s_2, s_3),$$
(2.26)

where  $p(s_1, s_2, s_3)$  is the underlying joint probability distribution.

The correlation functions,  $C_{ij}$ , can now be written in terms of the joint probability distribution  $p(s_1, s_2, s_3)$ :

$$C_{12} = p_{+++} + p_{++-} - p_{+-+} - p_{+--} - p_{-++} - p_{-+-} + p_{--+} + p_{---},$$
(2.27)

$$C_{23} = p_{+++} - p_{++-} - p_{+-+} + p_{+--} + p_{-++} - p_{-+-} - p_{--+} + p_{---},$$
(2.28)

$$C_{13} = p_{+++} - p_{++-} + p_{+-+} - p_{-++} + p_{-+-} - p_{--+} + p_{---}, \qquad (2.29)$$

where  $p_{+++}$  is the shorthand for p(+1, +1, +1), etc.

Consider the sum of  $C_{ij}$ :

$$C_{12} + C_{23} + C_{13} = 3p_{+++} - p_{++-} - p_{+-+} - p_{-++} - p_{-++} - p_{-++} - p_{--+} + 3p_{---}$$
  
= -1 + 4(p\_{+++} + p\_{---}) (2.30)

In the second line of the equation, we have used the fact that the sum of the probabilities over the entire sample space must equal one.

With a little rearranging, and the requirement that probabilities must be nonnegative, we immediately obtain the inequality:

$$1 + C_{12} + C_{13} + C_{23} \ge 0. \tag{2.31}$$

The rest of the LG3s can be found similarly by consider the following quantities:  $-C_{12} - C_{13} + C_{23}$ ,  $-C_{12} + C_{13} - C_{23}$  and  $C_{12} - C_{13} - C_{23}$ .

### 2.5 Families of LGIs

There are other LGIs that could be found when we consider different numbers of measurements.

First and foremost, there is the set of twelve two-time Leggett-Garg inequalities (LG2s) of the form:

$$1 + s_i \langle Q_i \rangle + s_j \langle Q_j \rangle + s_i s_j C_{ij} \ge 0, \tag{2.32}$$

where  $s_i$  has the usual meaning of the measurement outcome of variable Q at  $t = t_i$ . The LG2s are important because, as it turns out, the four LG3s alone are not sufficient for MR at three-time, the LG2s are a subset of conditions which are both necessary and sufficient for macrorealism at the three-time[17], just like Bell's inequalities to local realism (see also Chapter 3 for a full proof). We note here that for marcrorealism at two-time only, the LG2s serve as necessary and sufficient conditions.

Then we could also easily extend to find four-time Leggett-Garg inequalities, LG4s, which, just like LG3s to Bell inequalities, are of a similar structure to the CHSH inequalities. The LG4s consist of a total of eight inequalities of the form:

$$-2 \le C_{12} + C_{23} + C_{34} - C_{14} \le 2, \tag{2.33}$$

the other six inequalities can be found by moving the minus sign to three other possible locations. Notice the different pairing of the indices of the correlation functions compared to the CHSH inequalities.

Recall that during the derivation of LG3s (2.11)-(2.14) presented in the previous two subsections, we have noted that only the lower bound could be violated by quantum mechanics. The same is not true for the case of four-time. To see this, we consider the same two-level system as in the case of LG3s. Using equation (2.21), where we make the interval between consecutive measurements the same as before, then eight LG4s reduce to:

$$(LG4a) - 2 \le 3\cos(\omega t) + \cos(3\omega t) \le 2,$$
 (2.34)

$$-2 \le \cos(\omega t) + \cos(3\omega t) \le 2. \tag{2.35}$$

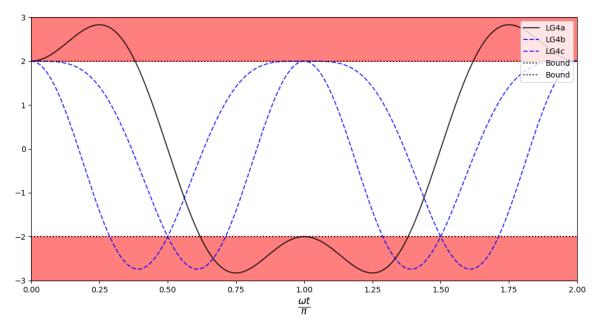
Where six of the LG4s reduce to inequality (2.35), and are always satisfied for all values of  $\omega t$ .

We can also generate new sets of inequalities by permutation of the time-indices. To be explicit, consider the following set of eight inequalities:

$$-2 \le C_{14} + C_{13} + C_{24} - C_{23} \le 2, \tag{2.36}$$

the rest can be found by moving the minus sign around, as before. This set of inequalities reduce to four more distinct inequalities which are not trivially satisfied:

$$(LG4b) - 2 \le \cos(3\omega t) + 2\cos(2\omega t) - \cos(\omega t) \le 2,$$
 (2.37)



**Figure 2.3:** A plot of the values of the LG4s, for a simple qubit-like system, same as **Figure 2.2**. Only the non-trivially satisfied inequalities are plotted here. The original form of LG4s only reduces to two inequalities, labelled LG4a (2.34), and represented by the solid black line . By considering other permutations of the time indices, we are able to find four more inequalities, labelled LG4b (2.37) and LG4c (2.38), plotted with blue dashed lines. Two things can be noticed in this plot: firstly, both the upper bound and the lower bound can be violated by the system; also, there are at least one inequality violated at all values of  $\omega t$ , except for multiples of  $\frac{\pi}{2}$ , which is also seen in the violation pattern of LG3s of the same system.

for the case of a minus sign being in front of  $C_{23}$ , and,

$$(LG4c) - 2 \le -\cos(3\omega t) + 2\cos(2\omega t) + \cos(\omega t) \le 2,$$
 (2.38)

for the case of a minus sign being in front of  $C_{14}$ .

Quantities in inequalities (2.34), (2.37), (2.38) are plotted as a function of  $\omega t$ , as shown in **Figure 2.3**. A few comments are in order. Firstly, notice that both bounds are violated by the system, therefore, both bounds are relevant and neither bound cannot be ignored completely, this also justified the counting of LG4s compared to LG3s, where we consider LG4s as eight inequalities and only four for the case of LG3s. It turns out that this is a general feature; both bounds are relevant when the number of measurement times is even, see equation (). Additionally, **Figure 2.3** shows the same violation pattern of the LG3s, i.e., LG4s are only satisfied at values of  $\omega t = \frac{\pi}{2}, \pi, \frac{3\pi}{2}$ , but this conclusion cannot be drawn if we only consider the original set of eight LG4s given by (2.33). This is a indication that the LG4s alone cannot be sufficient conditions for macrorealism, for we know that the system is not macrorealistic. Finally, as to the particular reason why no violations are found for  $\omega t$  equal to multiples of  $\frac{\pi}{2}$ , at the corresponding times, the state of the system is already an eigenstate of the measurement operator[18], and a QND measurement[19] is performed.

The forms of LG2s, LG3s and LG4s follow a particular pattern and can be generalized by the n-measurement Leggett-Garg strings[20]:

$$K_n = C_{12} + C_{23} + \dots + C_{(n-1)n} - C_{1n}.$$
(2.39)

Since each correlation function is bounded from above and below, e.g.,  $-1 \le C_{ij} \le 1$ , with  $\pm 1$  corresponding to perfect correlation and anti-correlation. We can then conclude that  $K_n$  is also bounded from above and below; by considering even and odd *n* separately, we arrive at the following formula for a family of LGIs:

$$-n \le K_n \le n-2 \qquad \text{for } n \ge 3, \text{ odd;} -(n-2) \le K_n \le n-2 \qquad \text{for } n \ge 4, \text{ even.}$$
(2.40)

In this formulation, we see that the set of LG3s we have been dealing with in the previous subsections are, in fact, the negative version of  $K_3$  considered here, which is, of course, mathematically equivalent. For the remaining of the paper, we will use the form of LG3s given by the formula (2.40) above for consistency. To be explicit, we redefine the LG3s to be:

$$-C_{12} - C_{23} - C_{13} \le 1 \tag{2.41}$$

$$C_{12} + C_{23} - C_{13} \le 1 \tag{2.42}$$

$$C_{12} - C_{23} + C_{13} \le 1 \tag{2.43}$$

$$-C_{12} + C_{23} + C_{13} \le 1 \tag{2.44}$$

Then, in our example of violations of LG3s, the only relevant bound is now the upper bound of 1, and this trend continues for all odd n, namely, only the upper bound of n - 2 for  $K_n$  is of interest. The LG4s given above are already of the form of the formula (2.40), and we stress again that for even n, both the upper bound and the lower bound could be potentially violated.

The Leggett-Garg strings do not, however, form complete sets of LGIs. We can utilize various symmetry properties [11] to derive further inequalities. If we redefine the variable Q to -Q independently at each time, the inequalities will still hold, this can be shown easily by considering **Table 2.3** and **2.4**. For a detailed example of this procedure, starting with  $K_3$ , with the minus sign originally in front  $C_{13}$  and corresponds to inequality (2.42), if we flip the sign of  $Q_1$  or  $Q_3$ , i.e., indices which one of the two correlation functions that having that index already has a minus sign in front, we then immediately obtain inequalities (2.43) and (2.44), which we note have the same number of minus signs as the inequality we started with. If we flip the sign of  $Q_2$ , i.e., indices which all related correlation functions are positive, we then obtain (2.41), which have two more minus signs. We can repeat this procedure for any n, and a set of inequalities will be completely found after we have considered all possible sign changes. Notice how the number of minus signs always goes up in twos, which means the number of minus signs in each inequality of a complete set of LGIs will always be an odd number. Also, for even n, inequalities with  $n_m$ 

minus signs are equivalent to those with  $n - n_m$  minus signs due to the fact that the inequalities are symmetric around 0.

Using the procedure described above, we can easily find complete sets of LGIs of any order. For the case of n = 4, it can be easily checked that the procedure yields the LG4s (2.33) given above. For n = 5, we will find that there are a total of 5 + 10 + 1 = 16 inequalities in the set of LG5s, with the numbers on the left corresponds to the number of inequalities found corresponding to the number of minus signs  $n_m = 1, 3, 5$  respectively.

However, as noted in later a later paper by Avis et al. [21], the LGIs found by the method above, for  $n \ge 4$ , are, in fact, reducible in the sense that they can be obtained by combining the original LG3s, which are referred to as triangle LGIs. The paper successfully shows the relation between LGIs and the facet inequalities for the geometry of cut polytopes[22]. In doing so, new irreducible LGIs can be found; particularly, for the case of n = 5, we have the "pentagon LGI",

$$\sum_{1 \le i \le j \le 5} C_{ij} + 2 \ge 0.$$
(2.45)

The pentagon inequality can be violated even when all the relevant LG3s are satisfied; see discussions in Chapter 4. This result does not, however, mean that the reducible higher-order LGIs are not interesting; there are situations in which their existence is useful, e.g., in addressing the clumsiness loophole[23].

## 2.6 Types of Measurements

The de Broglie-Bohm theory of quantum mechanics, as known as the "pilot wave" theory, by introducing new hidden variables, namely the position of the particles, to the wavefunctions while leaving the wavefunctions untouched, managed to reproduce all the standard experimental predictions of quantum mechanics and maintain the notion of realism at the same time. Based on this, Leggett, in his 2008 paper[10], has argued that:

[...], we shall never attempt to test realism alone, but always in conjunction with one or more other prima facie plausible assumptions about the world.

With this remark, in the case of macrorealism, the assumption of non-invasive measurability then becomes particularly important. As a side note, this justifies the name of the first assumption, macrorealism *per se*. Therefore, roughly speaking, macrorealism in the broader sense is a statement about the classical systems that observables process definite values at all times (realism) **and** measurements do not disturb the state of the system (NIM).

The requirement of non-invasive measurements, however, is challenging to implement experimentally; many experiments have done so, but achieving NIM always comes with arguments that are made dependent on the particular quantum system in question. In this section, we will review a few types of measurements that would, arguably, satisfy the NIM condition.

#### 2.6.1 Ideal Negative Measurement

Ideal negative measurements are proposed by Leggett and Garg in their original paper[1], as a method to satisfy non-invasiveness. When the detector measuring Q(t) in an experiment only interacts strongly with the system when the system is in one of the two possible states, e.g. Q(t) = +1, and does not interact at all otherwise, such measurements are considered to be ideal negative measurements.

If such detector is turned on at time t, and we do not get a response from the detector, we can then infer that the system at time t is in the state Q(t) = -1. In the limit of an arbitrarily short measurement, together with the assumption of MRps, it can be said that the measurement could not have affected the evolution of the system, thereby satisfying the assumption of NIM. In an experimental setting, where we measure the three correlation functions in different experiments, we could implement ideal negative measurements in the following way. In the experiment determining  $C_{ij}$ , we would need to measure the probabilities  $p_{ij}(s_i, s_j)$ . Since the dynamics of the system after  $t_j$  are not important, an ordinary (invasive) measurement can be performed at  $t_j$ , and an ideal negative measurement is performed at  $t_i$ . With the detector that only couples to the state  $Q_i = +1$ , we simply discard any runs with a response elicited by the system at  $t = t_i$ . In this way, we can obtain the value of  $p_{ij}(-1, s_j)$ . To obtain  $p_{ij}(+1, s_j)$ , we would then need a different detector

which couples only to the state  $Q_i = -1$ . In this way, we can, in the end, calculate the value of  $C_{ij}$  and continue to see if LG3s are indeed violated.

The testing protocol involving ideal negative measurements, as suggested above, is reasonable for the macrorealistic theories being put to the test, since they are inherently classical in nature[24]. It is, however, not compatible with quantum mechanics since a null result from such a detector still collapses the wavefunction[25]. This makes it challenging to identify the exact cause of violations of LGIs on quantum systems when utilizing ideal negative measurements, that which, if not all, of the assumptions, are not satisfied with the particular quantum system in question. Macrorealism does not assert that measurements cannot be invasive on a macrorealistic system, but rather it is possible for cleverly implemented measurements to avoid doing so. Therefore, a violation of the LGIs can indicate either (i) a violation of macrorealism by the system in question or (ii) the measurement protocol used in the experiment does disturb the system, which could still be macrorealistic in nature. (ii) is also known as the "clumsiness loophole"[23].

#### 2.6.2 Weak Measurements

In the quantum theory of measurement, a measurement involves the coupling between the object system, S, and the measurement apparatus, M, and the measured observable A is determined by the value of the pointer observable[26], R. The interaction between S and M is described by the Hamiltonian:

$$H = g(t)\hat{A} \otimes \hat{F} = g(t)AF,$$
(2.46)

where g(t) is called the instantaneous coupling rate and has non-zero values in the interval  $(t_i, t_f)$ , as interaction takes place, and  $\hat{F}$  is the operator of the "input" variable of M. At times,  $t \leq t_i$ , that the system, S, and the measurement apparatus, M, are uncorrelated and in the pure states  $|\psi\rangle$  and  $|\psi_M\rangle$  respectively. Then, for  $t \geq t_f$ , the states become correlated in this way:

$$|\psi_f\rangle = U|\psi\rangle|\psi_M\rangle,\tag{2.47}$$

by the unitary transformation,

$$U = exp(-i\int Hdt) = exp(-i\gamma AF), \qquad (2.48)$$

where  $\gamma$  is the coupling strength, defined to be,

$$\gamma = \int_{t_i}^{t_f} g(t) dt.$$
 (2.49)

Finally, a measurement of the "output" or the pointer variable, R, is taken at  $t \ge t_f$ , revealing information about the system. Note here we have ignored the free Hamiltonian of the system and the measuring apparatus for simplicity. When the coupling constant is sufficiently weak, we will refer to such measurements as weak measurements.

To be more explicit, we now suppose F and R are a pair canonically conjugate variables, say momentum, p, and position, q of a freely moving particle,

$$F = p, \qquad \qquad R = q. \tag{2.50}$$

Furthermore, we will assume that  $\hat{A}$  has discrete and non-degenerate eigenvalues,  $\alpha_i$ , such that we can expand  $|\psi\rangle$  as:

$$\psi = \sum_{j} \alpha_{j} |a_{j}\rangle, \tag{2.51}$$

where  $|a_j\rangle$  is the eigenstate of  $\hat{A}$  corresponding to the eigenvalue  $\alpha_j$ . We can then write equation (2.47) as:

$$\begin{split} |\psi_{f}(q)\rangle &\equiv \langle q|\psi_{f}\rangle = exp(-i\gamma\hat{A}\otimes p)\sum_{j}\alpha_{j}|a_{j}\rangle\psi_{M}(q) \\ &= \sum_{j}\alpha_{j}exp(-i\gamma a_{j}p)\psi_{M}(q)|a_{j}\rangle \\ &= \sum_{j}\alpha_{j}exp(-i\gamma a_{j}p)exp\left(-\frac{q^{2}}{4(\Delta q)^{2}}\right)|a_{j}\rangle \\ &= \sum_{j}\alpha_{j}exp\left(-\frac{(q-\gamma a_{j})^{2}}{4(\Delta q)^{2}}\right)\right)|a_{j}\rangle \\ &= \sum_{j}\alpha_{j}\psi_{M}(q-\gamma a_{j})|a_{j}\rangle \equiv \sum_{j}\alpha_{j}\psi_{M}(q_{f})|a_{j}\rangle, \end{split}$$
(2.52)

where  $\psi_M(q) = \langle q | \psi_M \rangle$  and  $q_f$  denotes the value of q at  $t \ge t_f$ . Also, as a reasonable assumption, we made  $|\psi_M\rangle$  a Gaussian in p (and consequently  $\psi_M(q)$ ). Then, after the interaction took place, we were left with a mixture of Gaussians located around  $\gamma a_j$ . In this way, it is clear that a projective measurement of q at,  $t \ge t_f$ , results in a projective measurement of A, when the wave packets  $\psi_M(q - \gamma a_j)$  do not overlap[27], that  $\gamma A = \delta q \equiv q_f - q$ . This imposes a condition on  $\gamma$  to be sufficiently strong:

$$|\gamma|(\delta a) \gg \Delta q, \tag{2.53}$$

where  $\delta a$  is the minimal distance between  $a_j$ 's and  $\Delta q$  is the uncertainty of q at  $t = 0 \le t_i$ .

When the condition (2.53) is not met, however, such measurements (weak measurements) provide almost no information since the uncertainty in the measurement is too big. We are still able to measure the expectation value,  $\langle A \rangle$ , since, from equation (2.52), we have:

$$\langle q_f \rangle - \langle q \rangle = \gamma \langle A \rangle,$$
 (2.54)

by performing multiple runs of the same experiment, effectively decreasing the uncertainty  $\Delta q$ . By increasing the number of repeats, we can determine  $\langle A \rangle$  to any desired precision.

In summary, weak measurements measure the expectation value,

$$\langle A \rangle = \sum_{j} |\alpha_j|^2 a_j = \sum_{j} p_j(a_j) a_j, \qquad (2.55)$$

very differently to projective measurements. When using projective measurements, we measure the probabilities,  $p_j(a_j)$ , directly in experiments to then calculate the expectation value. On the other hand, the expectation value is obtained by equation (2.54) directly in the case of weak measurements.

We note that in the original paper by Leggett and Garg, it is implicit that the quantities  $Q_i$  are to be obtained using projective measurements. Either type of measurement we use in an experiment, the quantum correlation function, equation (2.20), remains in the same form[13]. Therefore, we can replace the projective measurements in the standard protocol for LGIs, with weak measurements, i.e., obtaining the correlation functions in three separate experiments using weak measurements, without having to worry too much about the consequences (this argument does not necessarily hold for systems of larger dimension[11; 28]). We can then conclude that the standard protocol, as discussed above, referred to as the *two-point* method, is independent of measurement strength[11].

We note here that the benefit of using weak measurements is that the wavefunction of the system is only partially collapsed by a weak measurement, when carefully implemented, with the trade off being less information can be extracted from a single measurement. In the limit of a true weak measurement, i.e.,  $\gamma \rightarrow 0$ , there is a vanishing effect on the wavefunction of the system, which one hopes would satisfy the NIM condition and avoid the clumsiness loophole; this is, however, extremely hard to achieve experimentally, as expected.

The name of the two-point protocol refers to the fact that the system is only measured at two out of three possible points in time in any run. In contrast, a three*point* protocol can be designed, where measurements at all three points in time are performed[29]. In this protocol, only the second measurement needs to be weak since the first measurement can also be considered as fixing the initial state of the system, and, same as before, the evolution of the system is irrelevant after the third measurement[30]. Repeated runs of a such experiment will give us the probability distribution  $p(s_1, q_2, s_3)$ , where  $s_1$  and  $s_3$  have the usual meaning of the outcome of a projective measurement of the value  $Q_1$  and  $Q_3$ , and  $q_2$  is the outcome obtained from the weak measurement at  $t = t_2$ . Note that  $q_2$  here is different to the pointer variable q in equation (2.50)-(2.54), it corresponds to the response of the ambiguous detector performing the weak measurement, also called the *contextual value* of the variable  $Q_2$ [31], defined such that the expectation,  $\langle q_2 \rangle \equiv \int dq_2 q_2 p(q_2)$ , is consistent with the expectation value with that of a projective measurement of  $Q_2$ . By only considering the case,  $s_1 = +1$ , thought of as setting the initial state of the system in  $Q_1 = +1$ , then the left-hand side of equation (2.42) can be written as[30]:

$$K_{3} = \langle q_{2} \rangle + \langle q_{2}Q_{3} \rangle - \langle Q_{3} \rangle$$
  
=  $\sum_{s_{3}=\pm 1} \int dq_{2}p(q_{2}, s_{3})(q_{2} + s_{3}q_{2} - s_{3}) \leq 1,$  (2.56)

where we have used the fact that  $p(s_1, q_2, s_3) = p(q_2, s_3)\delta_{s_1,+1}$ . Note that the sum over  $s_2$  when the measurement at  $t = t_2$  has been replaced with a integral over  $q_2$ ; this is due to the fact that the pointer variable  $q_2$  could be continuous, and the range of  $q_2$  necessarily exceeds the range of the system variable  $Q_2$ [11], this is ab interesting property of the contextual values when using weak measurements.

It can be shown that in the limit of  $\gamma \to \infty$ , inequality (2.56) is always satisfied. This is consistent with the remark made on inequality (2.18). However, in the opposite limit, as  $\gamma \to 0$ , the upper bound of unity can be violated. In the particular example of a spin- $\frac{1}{2}$  particle given above, maximum violation of inequality (2.56) with the same pattern of violations occur as  $\gamma \to 0$ [11]. Therefore, for any  $\gamma$  in the range  $[0, \infty)$ , inequality (2.56) can be violated.

It is worth noting that the two-point and three-point protocols admit violations of LGIs in opposite ways. Following the two-point protocol, we obtain the three independently measured two-point correlation functions and assume the existence of a joint probability distribution that is compatible with the correlation functions. Failing to find such a joint probability distribution is the root source of the violation of LGIs in the two-point case. Whereas in the three-point case, we obtain the joint probability distribution  $p(s_1, q_2, s_3)$  directly, and then to find that the marginal probabilities (see Chapter 3) calculated from the measured joint probability distribution are not compatible with the NIM assumption or each other. In this way, inequality (2.56) can be violated.

#### 2.6.3 Continuous Weak Measurements

Another way to implement weak measurements in testing quantum systems for macrorealism is *continuous weak measurements*, particularly useful when a detector is permanently attached to the system. Here we follow the arguments given by Ruskove et al.[32] and show that the occurrence of violations of LGIs in a quantum stochastic approach.

When making continuous weak measurements on a system, instead of measuring the value of  $Q_i$  directly, the detector shows a noisy signal:

$$I(t) = I_0 + \frac{\Delta I}{2}Q(t) + \xi(t), \qquad (2.57)$$

where  $I_0$  is a constant offset to the signal due to background,  $\Delta I$  is the difference in the signal corresponding to the state Q(t) = +1 and Q(t) = -1, and  $\xi(t)$  represents the Gaussian white noise present in the system that is stochastic in nature. The variable  $\xi(t)$  has a vanishing temporal average,

$$\langle \xi(t) \rangle \equiv \lim_{T \to \infty} \frac{1}{T} \int_{-T/2}^{t} T/2 dt \xi(t) = 0,$$
 (2.58)

and a  $\delta\text{-function}$  correlator,

$$\langle \xi(t)\xi(t+\tau)\rangle = \frac{S_0}{2}\delta_{\tau},$$
(2.59)

where  $\tau$  is a arbitrary time interval such that  $\tau > 0$ , and  $S_0$  is the spectral density. The symbol I(t) originated from measurement apparatus such as a quantum point contact (QPC)[33], where the signal is a current. By averaging I(t), one obtains:

$$C_{I}(\tau) = \langle [I(t) - I_{0}][I(t+\tau) - I_{0}] \rangle$$
  
=  $\left(\frac{\Delta I}{2}\right)^{2} \langle Q(t)Q(t+\tau) \rangle + \left(\frac{\Delta I}{2}\right) (\langle \xi(t)Q(t+\tau) \rangle + \langle Q(t)\xi(t+\tau) \rangle),$  (2.60)

where the second line is obtained by substituting equations (2.58) and (2.59). Under the assumptions of NIM and induction, we can assume that the state of the system at time t cannot affect future noise in the detector and that the noise registered by the detector at time t does not disturb the subsequent measurements of variable  $Q(t+\tau)$ , therefore the following correlators must have a value of zero,

$$\langle \xi(t)Q(t+\tau)\rangle = \langle Q(t)\xi(t+\tau)\rangle = 0, \qquad (2.61)$$

for a macrorealistic system.

By combining equations (2.60), (2.61) and the LGI (2.42), we obtain an inequality for the correlation functions of the detector signal:

$$C_I(t_2 - t_1) + C_I(t_3 - t_2) - C_I(t_3 - t_1) \le 1 \times \left(\frac{\Delta I}{2}\right)^2.$$
 (2.62)

The experimental benefit of this protocol is that the experiment only needs to be run once. Experiments have been performed[32], and violations of the inequality are, of no surprise, found in quantum systems. It is argued that this protocol still has not managed to avoid the clumsiness loophole[23], but simply rephrased in the form of equation (2.61), that the reason inequality (2.62) is violated is that the system inevitably feels a backaction from the detector such that  $\langle \xi(t)Q(t+\tau)\rangle \neq 0$ .

#### 2.6.4 Continuous In Time Velocity Measurements

A different approach to testing the LGIs is proposed by JJ Halliwell in 2016[24], which bears a resemblance to both continuous weak and ideal negative measurements, which could be implemented in a way that presents a stronger argument for its non-invasiveness in both classical theories and quantum mechanics.

The protocol is conceptually straightforward, and consists of a single "waiting detector" weakly coupled to the system, which only registers a click when the variable Q(t) changes sign. This is motivated by the observation that the correlation functions can be written as,

$$C_{ij} = p(Q_i = Q_j) - p(Q_i \neq Q_j),$$
 (2.63)

that the correlation function only depends on whether the observable, Q(t), has the same value (sign) or not at times  $t = t_i$  and  $t = t_j$ . We can then rephrase equation (2.63) as:

$$C_{ij} = 1 - \frac{1}{2} \left\langle [Q_j - Q_i]^2 \right\rangle,$$
 (2.64)

which is consistent with both the classical definition (2.10) and the quantum analogue (2.20). Further more, we will assume the existence of a velocity variable,  $v(t) = \dot{Q}(t)$ , such that,

$$Q_j - Q_i = \int_{t_i}^{t_j} dt v(t),$$
(2.65)

and can be experimentally measured by an ancilla weakly coupled to the system. We note that the existence of such variables is not normally assumed by the LGI framework; however, there are quantum systems in which such a velocity is readily identified, for example, for the spin- $\frac{1}{2}$  particle system considered many times in this chapter, the velocity is defined as  $\dot{\sigma}_z = \omega \sigma_y$ .

For simplicity, we will now present the quantum mechanical implementation of the protocol using the aforementioned spin- $\frac{1}{2}$  system (S), and additionally, a two-state ancilla (A) weakly coupled to v(t) of S. The total Hamiltonian of the system is then written as (ignoring hats):

$$H = \left(\frac{1}{2}\omega\sigma_x\right) \otimes \mathbb{1} + \gamma(\omega\sigma_y) \otimes (|0\rangle\langle 1| + |1\rangle\langle 0|),$$
(2.66)

where it is clear that operators to the left of the tensor products act on S and the opposite acts on A, and  $\gamma$  is the coupling strength as discussed above. The ancilla is initialized in the state  $|0\rangle$  and will flip to the state  $|1\rangle$  when an interaction takes place.

By noting that  $H^2 = (\Omega^2/4)\mathbb{1} \otimes \mathbb{1}$ , where  $\Omega = \omega \sqrt{1 + 4\gamma}$ , we can Taylor expand the unitary time evolution operator as:

$$U(t) = exp(-iHt) = \cos\left(\frac{\Omega t}{2}\right) \mathbb{1} - \frac{2i}{\Omega}\sin\left(\frac{\Omega t}{2}\right) H.$$
 (2.67)

Then for a general state at time t, we can write:

$$\begin{aligned} |\Psi(t)\rangle &= U(t)(|\psi\rangle \otimes |0\rangle) \\ &= (A_0(t)|\psi\rangle) \otimes |0\rangle + (A_1(t)|\psi\rangle) \otimes |1\rangle, \end{aligned}$$
(2.68)

where,

$$A_0(t) = \cos\left(\frac{\Omega t}{2}\right) \mathbb{1} - \frac{i\omega}{\Omega} \sin\left(\frac{\Omega t}{2}\right) \sigma_x,$$
(2.69)

and,

$$A_1(t) = -\frac{2i\gamma\omega}{\Omega} \sin\left(\frac{\Omega t}{2}\right)\sigma_y,$$
(2.70)

found by simple expansion.

We can then calculate the probability of finding the ancilla in state  $|1\rangle$ :

$$p(1) = \langle \psi | A_1^{\dagger}(t) A_1(t) | \psi \rangle$$
  
=  $\frac{2\gamma^2 \omega^2}{\Omega^2} [1 - \cos(\Omega t)].$  (2.71)

In the weak measurement limit, we assume  $\gamma \ll 1$ , so that  $\Omega \approx \omega$ , and p(1) becomes:

$$p(1) \approx 2\gamma^2 [1 - \cos(\omega t)] = 2\gamma^2 (1 - C_{ij}),$$
 (2.72)

where  $C_{ij} = cos(\omega t)$  for  $t_j - t_i = t$ . It is also worth checking that,

$$p(0) = \langle \psi | A_0^{\dagger}(t) A_0(t) | \psi \rangle$$
  

$$\approx 1 - 2\gamma^2 (1 - C_{ij}) = 1 - p(1),$$
(2.73)

as expected.

It is noted that measurement p(1) and p(0) are not the same as  $p(s_i = s_j)$  and  $p(s_i \neq s_j)$  as in equation (2.63), in fact, they are related by:

$$p(1) = 4\gamma^2 p(s_i \neq s_j),$$
  

$$p(0) = p(s_i = s_j) + (1 - 4\gamma^2) p(s_i \neq s_j),$$
(2.74)

which can be thought of as that only a  $4\gamma^2$  fraction of sign changes is detected by the ancilla due to the fact the ancilla is only weakly coupled to the system.

There is a crucial requirement for this measurement protocol to work as intended. Namely, we will need to limit the time interval t so that the system, under free evolution, can undergo at most one sign change within that time. This requirement has several reasoning behind it. The first is that the ancilla cannot distinguish between zero and two sign changes since the second sign change will make the state of the ancilla back to  $|0\rangle$ . Secondly, assume the time interval is short enough for one sign change at most. Then, if the ancilla is found in the  $|0\rangle$  state, there are only two possible explanations: (i) the system variable Q has not changed sign during the time interval, (ii) the ancilla changes state as the sign of Q flipped, but the back action from the ancilla caused the sign to flip a second time, which then interacts with the ancilla a second time, causing the state to change back to the initial state  $|0\rangle$ . One could argue for the non-invasiveness of the protocol if case (ii) has a vanishing probability of happening compared to case (i). This probability can, in fact, be calculated explicitly using the equations above; the probability that ancilla has a history of  $|0\rangle \rightarrow |1\rangle \rightarrow |0\rangle$  at times 0, t, 2t (for simplicity), is given by,

$$p_{010} = A_1^4(t) = \frac{16\gamma^4 \omega^4}{\Omega^4} \sin^4\left(\frac{\Omega t}{2}\right)$$

$$\approx 16\gamma^4 \sin^4(\frac{\omega t}{2}),$$
(2.75)

which is just the square of the probability of a single sign change given by (2.71), under the same assumption that  $\Omega \approx \omega$ . In contrast, case (i) has a probability,  $p_{011}$ , given by,

$$p_{011} = A_1^2(t)A_0^2(t) = \frac{4\gamma^2\omega^2}{\Omega^2}\sin^2\left(\frac{\Omega t}{2}\right) \left[\cos^2\left(\frac{\Omega t}{2}\right) + \frac{\omega^2}{\Omega^2}\sin^2\left(\frac{\Omega t}{2}\right)\right]$$

$$\approx 4\gamma^2 \sin^2(\omega t).$$
(2.76)

By inspection, it is easy to see that  $p_{010}$  is of a factor of  $\gamma^2$  smaller than  $p_{011}$ , since we are already assuming  $\gamma \ll 1$ . Furthermore, we could test for disturbances if the final state of ancilla is found to be  $|0\rangle$  by performing a measurement at some time after  $t_f$  and comparing the outcome with the initial state of the system S which would be fixed. We now consider case when the ancilla is in state  $|1\rangle$  at time  $t_f$ . In this case, it is clear that the sign of Q must have flipped once as it would under free evolution of the system S, since no interaction can happen between the ancilla and the system before the sign flip. The interaction with the ancilla could then cause either (i) no disturbance, (ii) some non-zero back action but no sign flipping as a result, or (iii) some non-zero back action and flipping the sign a second time. Case (iii) has already been considered, whereas case (ii) does not have an effect on the correlation functions when the system is measured in this way. Therefore, we can conclude that with this particular set-up, at least, when the coupling strength is sufficiently small and the time interval is sufficiently short, back action from the ancilla can be statistically ignored, that the protocol satisfies the NIM condition, to a good approximation. It is then proved by Halliwell[24] that such a short time scale assumption, where Q only changes sign once, is reasonable in both classical and quantum formulations.

Experiments utilizing this protocol have already been performed [34], and they have shown that the results of the CTVM protocol agreed with those of the ideal negative protocol and admit the violations of LGIs.

### 2.7 Summary

We first began this chapter by reviewing the EPR paradox, arguments made by Einstein et al. for the existence of local realism against the Copenhagen interpretation of quantum mechanics. This is as expected since concepts implied by the Copenhagen interpretation were hard to accept by almost anyone at the time, and the intuitions we developed on the physical world were profoundly challenged. To resolve the disputes, Bell then proposed a more sophisticated experimental set-up and derived a set of inequalities which would be satisfied if the assumptions of local realism were indeed correct. Backed by experimental data, the notion of local realism is then violated by a variety of quantum systems through the Bell/CHSH framework.

This all served as motivation to Leggett and Garg, who proposed the notion of macrorealism in their original paper in 1985, along with it, a set of Leggett-Garg inequalities which could be satisfied if a given system is so-called macrorealistic. The set of LGIs, in most literature, is considered to be the temporal version of Bell inequalities, although it could be argued that the LGIs are a generalization of the Bell inequalities as they are less restrictive in the types of systems they can apply to. As noted by Leggett, realism should always be tested in conjunction with other logical assumptions about the physical reality; in the case of macrorealism, it is the ability to perform measurements on a particular system without disturbing the system's evolution at test. Violation of macrorealism implies that a classical view of the system must be abandoned, that the system exhibits "quantumness". In this way, the LGIs are particularly useful in the journey towards achieving macroscopic coherence and explorations of the boundaries of the classical limit.

In sections 2.4 and 2.5, we reviewed a few of the many derivations of the LGIs as well as other forms of the LGIs. We note here that sets of LGIs in the form of equation (2.39) for  $n \ge 3$  measurements are not yet complete, in that LG3s, LG4s, or higher-order LGIs alone cannot be viewed as necessary and sufficient conditions for MR at the corresponding measurement times. We will present the proof of Fine's theorem and use it as a guide to complete the LG framework in Chapter 3.

Much of the current experimental work is focused on, arguably, not-macroscopic systems, where the goal is to understand the patterns better and identify the cause of violations of the LGIs. In these quantum systems, it is the condition of NIM that is the most challenging to implement, and it always comes with assumptions that are dependent on the particular system being tested. These assumptions, or arguments, do not hold in general cases since quantum mechanical measurements are always invasive to some degree. Different protocols with different measurement schemes have been proposed and experimented with, as discussed in section 2.6. However, the problem, known as the clumsiness loophole, remains, that a macrorealist could always view the violations of LGIs as failure to satisfy NIM such that MRps cannot be refuted by the violations. It is argued that, unless there is a way to close this loophole, the LG framework for testing macrorealism is not methodologically on par with the Bell/CHSH framework. More discussion on this will follow.

## Chapter 3

## **Conditions for Macrorealism**

### 3.1 Fine's Theorem

#### 3.1.1 Marginal Probabilities

First, we consider a simple system with two variables with measurement outcomes,  $s_1$  and  $s_2$ , such that  $s_i \in \{\pm 1\}$ . There are then  $2^2 = 4$  possible combinations of measurement outcomes  $(s_1, s_2)$  each with some probability  $p_{12}(s_1, s_2)$  of occurring, we call these probabilities pairwise probabilities. These four pairwise probabilities must satisfy the following relation,

$$\sum_{s_1, s_2=\pm 1} p_{12}(s_1, s_2) = 1, \tag{3.1}$$

since the system is completely described by these two variables, therefore the union of the four combinations must equal the entire sample space. For this simple twovariable system, the pairwise probabilities  $p_{12}(s_1, s_2)$  are the *underlying probability distribution* of the system. Given the underlying probability distribution, we can find different *marginal probabilities* of the system, defined as the probability of an event happening independent of other events. In this case, by summing over one of the systems variables  $s_i$ , we can find the marginal probabilities  $p_j(s_j)$  for  $i \neq j$ , e.g.

$$p_1(s_1) = \sum_{s_2=\pm 1} p_{12}(s_1, s_2).$$
 (3.2)

See Table 3.1 for a detailed description of the system.

This notion of an underlying and marginal probability distribution can easily extend to systems with more variables. For a system with n variables with n measurement outcomes, the underlying probability distribution will be labelled as  $p_{12...n}(s_1, s_2, ..., s_n)$ .

In the experimental set-up for CHSH inequalities, the system concerns four variables with measurement outcomes,  $s_1$ ,  $s_2$ ,  $s_3$  and  $s_4$ , namely the spins of two entangled particles measured along one of two axes, where each measurement outcome,

	$s_1 = +1$	$s_1 = -1$	Row Sum
$s_2 = +1$	$p_{12}(+1,+1)$	$p_{12}(-1,+1)$	$p_2(+1)$
$s_2 = -1$	$p_{12}(+1,-1)$	$p_{12}(-1,-1)$	$p_2(-1)$
Column Sum	$p_1(+1)$	$p_1(-1)$	

Table 3.1: Marginal probabilities

just like the example above, can take values of  $\pm 1$ . If the local hidden variables theory is indeed the correct description of the system, such that there exist a set of hidden variables matching the pairwise probabilities,  $p_{13}(s_1, s_3)$ ,  $p_{14}(s_1, s_4)$ ,  $p_{23}(s_2, s_3)$ and  $p_{24}(s_2, s_4)$ , measured indirectly in the experiment, then it is clear that an underlying probability distribution,  $p_{1234}(s_1, s_2, s_3, s_4)$ , must exist. Additionally, the pairwise probabilities can then be thought of as the marginal probabilities of the system, and they can be obtained by summing over the corresponding outcomes. As we discussed in Chapter 2, the existence of such underlying probability is a necessary condition for establishing bounds on the correlation functions, which in turn gives us the CHSH inequalities. Violating the CHSH inequalities must then imply that the assumption of the existence of an underlying probability distribution is incorrect. We can, therefore, conclude that CHSH inequalities are a necessary condition for local realism.

#### 3.1.2 Proof of Fine's Theorem

The derivation of CHSH inequalities, however, does not prove the opposite, that satisfaction of the CHSH inequalities must imply the existence of an underlying probability distribution. In other words, we have not yet proved that satisfying the CHSH inequalities is not only a necessary condition for local realism, but it is also a sufficient one. At its core, validating realism is all about proving the existence of an underlying probability distribution. This is the exact problem Fine's theorem addressed.

In his paper, Arthur Fine has proved that the following five statements about a quantum correlation experiment are equivalent[6]:

- 1. There is a deterministic local hidden-variables model for the experiment.
- 2. There is a factorizable, stochastic model for the experiment.
- 3. There exists one joint distribution for all observables of the experiment, whose marginals match the probabilities obtained from the experiment.
- 4. There are well-defined, compatible joint distributions for all pairs and triples of commuting and non-commuting observables.
- 5. The Bell/CHSH inequalities hold.

Here we note that the conclusion we desire, namely that CHSH and Bell inequalities are both necessary and sufficient conditions for local realism, is only one of the results of Fine's theorem. Fine's original proof is purely algebraic and not as immediately apparent as the proof of necessity. For these reasons, this review will not cover the full proof. Instead, we will follow a perhaps simpler proof by JJ Halliwell[35] for the case of Bell's inequalities, which, as we will see later, is closely related to the Leggett-Garg inequalities we have been discussing.

Consider a system with three variables, and we have obtained the three pairwise marginal probabilities,  $p_{12}(s_1, s_2)$ ,  $p_{23}(s_2, s_3)$  and  $p_{13}(s_1, s_3)$ . The underlying probability distribution,  $p_{123}(s_1, s_2, s_3)$ , may be written as:

$$p_{123}(s_1, s_2, s_3) = \frac{1}{8} \left( 1 + \sum_i B_i s_i + \sum_{i < j} C_{ij} s_i s_j + D s_1 s_2 s_3 \right),$$
(3.3)

where the indices i, j, k run over the values 1, 2, 3, and the correlation functions  $B_i$ ,  $C_{ij}$  and D are found by:

$$B_i = \sum_{s_1, s_2, s_3} s_i p_{123}(s_1, s_2, s_3), \tag{3.4}$$

$$C_{ij} = \sum_{s_1, s_2, s_3} s_i s_j p_{123}(s_1, s_2, s_3),$$
(3.5)

$$D = \sum_{s_1, s_2, s_3} s_1 s_2 s_3 p_{123}(s_1, s_2, s_3).$$
(3.6)

The marginal probabilities in this form are then easily found by summing over  $s_i$ , e.g.

$$p_{13}(s_1, s_3) = \sum_{s_2=\pm 1} p_{123}(s_1, s_2, s_3) = \frac{1}{4} \left( 1 + B_1 s_1 + B_3 s_3 + C_{13} s_1 s_3 \right).$$
(3.7)

There are a total of  $3 \times 4 = 12$  equations of this form, and they relate functions  $B_i$  and  $C_{ij}$  with marginal probabilities that we have already obtained. Therefore, by knowing the marginal probabilities. we completely fix  $B_i$  and  $C_{ij}$ .

By requiring the marginal probabilities are non-negative, we immediately obtain a set of twelve inequalities from equation (3.7):

$$1 + B_i s_i + B_j s_j + C_{ij} s_i s_j \ge 0.$$
(3.8)

These conditions are trivially satisfied since we have already obtained the marginal probabilities.

Additionally, equation (3.3) is also required to be non-negative. Since we have fixed  $B_i$  and  $C_{ij}$ , the only free parameter is D, and we can therefore obtain the following inequality:

$$A(s_1, s_2, s_3) \equiv \left(1 + \sum_i B_i s_i + \sum_{i < j} C_{ij} s_i s_j\right) \ge -Ds_1 s_2 s_3.$$
(3.9)

For the case  $s_1s_2s_3 = 1$ , we obtain four lower bounds for *D*:

$$-A(s_1, s_2, s_3) \le D. \tag{3.10}$$

For the case  $s_1s_2s_3 = -1$ , we obtain four upper bounds for *D*:

$$A(s_1, s_2, s_3) \ge D. \tag{3.11}$$

Thus, D will exist as long as the lower bounds are indeed lower than the upper bounds. We, therefore, obtain constraints of the form:

$$-A(+1,+1,+1), -A(+1,-1,-1), -A(-1,+1,-1), -A(-1,-1,+1) \\ \leq A(+1,+1,-1), A(+1,-1,+1), A(-1,+1,+1), A(-1,-1,-1).$$
(3.12)

There are a total of sixteen inequalities. Depending on the relation between the arguments of both sides, they group into two sets of inequalities. One set is found by pairing up those with two arguments being the same, e.g.,

$$-A(+1,-1,-1) \le A(+1,-1,+1) \Rightarrow 1 + B_1 - B_2 - C_{12} \ge 0.$$
(3.13)

In this case, both sides have  $s_1 = +1$  and  $s_2 = -1$ , and we obtain the same inequality as we would from equation (3.8) by requiring  $p_{12}(+1, -1)$  to be non-negative. Therefore, twelve of the sixteen inequalities in equation (3.12) are already found by requiring the marginal probabilities to be non-negative.

The set of four new inequalities is found by pairing up those with all three arguments being opposite:

$$-A(+1,-1,-1) \le A(-1,+1,+1) \Rightarrow +C_{12} + C_{13} - C_{23} \le 1,$$
(3.14)

$$-A(+1,-1,-1) \le A(+1,-1,+1) \Rightarrow +C_{12} - C_{13} + C_{23} \le 1,$$
(3.15)

$$-A(-1,-1,+1) \le A(+1,+1,-1) \Rightarrow -C_{12} + C_{13} + C_{23} \le 1,$$
(3.16)

$$-A(+1,+1,+1) \le A(-1,-1,-1) \Rightarrow -C_{12} - C_{13} - C_{23} \le 1.$$
(3.17)

These are, in fact, a form of Bell's original inequalities[36]. We have thus shown that by requiring the existence of an underlying probability distribution, i.e.,  $p_{123}(s_1, s_2, s_3) \ge$ 0, Bell's inequalities follow. Most importantly, since inequalities of the form of (3.13) are guaranteed to be satisfied, and there are no further restrictions other than Bell's inequalities, we can now conclude that satisfaction of Bell's inequalities is a sufficient condition for ensuring the existence of an underlying probability. Combining with the discussions above, we have now proven that Bell's inequalities are necessary and sufficient conditions for local realism.

#### 3.1.3 Generalized Fine Ansatz

We can extend the proof in the last subsection to measurements at more times. Specifically, when dealing with measurements at four times, our goal is to find the set of necessary and sufficient conditions for the existence of the four-time probability distribution,  $p_{1234}(s_1, s_2, s_3, s_4)$ , matching the four known two-time marginal probabilities,  $p_{13}(s_1, s_3)$ ,  $p_{14}(s_1, s_4)$ ,  $p_{23}(s_2, s_3)$  and  $p_{24}(s_2, s_4)$ , and we fully expect the conditions found are of the form of CHSH inequalities (2.7). In proving sufficiency, we encounter the difficulty that only four of the six possible marginals are fixed in this problem. It is proposed that the matching problem can be solved using the following Fine's ansatz[37]:

$$p(s_1, s_2, s_3, s_4) = \frac{p(s_1, s_2, s_3)p(s_1, s_2, s_4)}{p(s_1, s_2)},$$
(3.18)

where we have ignored the subscripts for simplicity. This simplifies the problem of proving the existence of the two three-time probabilities and one two-time probability, which we have already seen that the resulting conditions are in the form of inequalities (3.8) and the Bell-type inequalities (3.14)-(3.17).

As we have noted before, the LG4s are similar to CHSH inequalities but with a different pairing of measurements. For the LG test at four times then, the ansatz becomes:

$$p(s_1, s_2, s_3, s_4) = \frac{p(s_1, s_2, s_3)p(s_1, s_3, s_4)}{p(s_1, s_3)}.$$
(3.19)

This can be generalized to any number of measurement times [37], specifically, for n-time, we have:

$$p(s_1, ..., s_n) = \frac{p(s_1, ..., s_{n-1})p(s_1, s_{n-1}, s_n)}{p(s_1, s_{n-1})},$$
(3.20)

and we are left with a n-1-time probability, a three-time probability and a two-time probability. We can then apply the n-1-time ansatz and so on to finally obtain the formula for generalized Fine's ansatz:

$$p(s_1, \dots, s_n) = p(s_1, s_2, s_3) \prod_{i=1}^{n-3} \frac{p(s_1, s_{i+2}, s_{i+3})}{p(s_1, s_{i+2})}.$$
(3.21)

This formula provides another way of finding LG*n*s and implies that we can always reduce a *n*-time problem to a set of three-time problems. This is consistent with the finding by Avis et al.[21] as we have noted in section 2.5 that the LGIs are reducible for  $n \ge 4$ . Most importantly, with the help of the generalized Fine ansatz, we can easily extend our existing framework to measurements at more times, lifting the restrictions on how we test the system.

## **3.2 Sufficient Conditions for MR**

We now return to the discussion of the Leggett-Garg inequalities. As we have discussed in Chapter 2, the Leggett-Garg inequalities were designed by analogy with the Bell inequalities and often considered to be a temporal version of the Bell inequalities. However, Maroney and Timpson [12] in their paper argued that Bell and LG tests are not methodologically on par due to fact that the assumption of noninvasive measurability cannot be made suitably model-independent. Nevertheless, our goal here is to modify the proposed LG framework and construct a decisive test for macrorealism just like the Bell inequalities to local realism, as Fine's theorem has proved.

Depending on the measurement protocol used in various experiments, there exists different *interpretations* of the NIM assumption[17]. In the original LG framework, for example, the correlation functions are obtained from three separate experiments, where each experiment only measures at two of the times, and we only require that NIM is satisfied in each experiment, i.e., two sequential measurements only. We will denote this piecewise interpretation as NIM<sub>pw</sub>. However, some protocols assume a different interpretation of NIM, where it is required that the system is undisturbed by *any* number of sequential measurements in a single experiment. We will denote this interpretation as NIM<sub>seq</sub>. It is then clear that NIM<sub>seq</sub> is a stronger notion than NIM<sub>pw</sub>, for that a set-up which satisfy NIM<sub>pw</sub> may not satisfy NIM<sub>seq</sub>. It is argued by Halliwell[17] that there exist different versions of MR, depending on which interpretation of NIM is assumed, and the set of necessary and sufficient conditions also varies for different versions of MR. Explicitly, using the same notation as Halliwell's paper, we will denote these two versions as MR<sub>weak</sub> and MR<sub>strong</sub>.

In Bell experiments, there are a set of trivial conditions that the pairwise probabilities must satisfy, which we have not mentioned in the last subsection. They are of the form:

$$\sum_{s_1} p_{12}(s_1, s_2) = p_2(s_2).$$
(3.22)

Such conditions ensure that the pairwise probabilities,  $p_{12}(s_1, s_2)$ ,  $p_{13}(s_1, s_3)$  and  $p_{23}(s_2, s_3)$ , are compatible with each other. These are guaranteed by causality since there cannot be any signalling between the two spacelike separated detectors. However, the same cannot be said for the case of LG experiments; since measurements are timelike separated, equation (3.18) is not generally satisfied. In the context of the LG framework, conditions in equation (3.18) are referred to as *No Signalling In Time* (NSIT) conditions in analogy to the no signalling in Bell experiments, and they are closely related to the implementation of NIM. This is a crucial distinction between the LG and Bell framework, and equation (3.18) must be satisfied in order for Fine's theorem to apply.

#### 3.2.1 Augmented LG Framework

The two-time probabilities, similar to equation (3.7), in an LG-like set-up, can be constructed as:

$$p(s_i, s_j) = \frac{1}{4} (1 + s_i \langle Q_i \rangle + s_j \langle Q_j \rangle + s_i s_j C_{ij}).$$
(3.23)

We note two changes. Firstly, we have replaced the correlation functions  $B_i$  with the averages  $\langle Q_i \rangle$  for clarity. The second is that we have removed the subscript on the two-time probabilities, which were used to denote which measurements were taken in obtaining it. It is clear from the formula that we need the quantities  $\langle Q_i \rangle$  to compute the probabilities. In certain protocols, like with ideal negative measurements, the two-time probabilities are measured directly, from which we could read off  $C_{ij}$  and  $\langle Q_i \rangle$ , we would then label the probabilities with the corresponding subscripts. However, there exist non-invasive protocols in which only the correlation functions  $C_{ij}$  are measured in a single experiment [17], and measuring  $\langle Q_i \rangle$  in different experiments clearly satisfies NIM since only one measurement is taken. Hence, to be more general, we instead assume that  $C_{ij}$  and  $\langle Q_i \rangle$  are measured in six separate experiments to best satisfy the NIM<sub>pw</sub> requirement.

From equation (3.19), it is then clear that the following conditions are trivially satisfied:

$$\sum_{s_i} p(s_i, s_j) = p(s_j) = \sum_{s_k} p(s_j, s_k),$$
(3.24)

provided that  $\langle Q_i \rangle$  are measured in separate experiments. Here we note a subtle point: even though these equations are mathematically equivalent to the NSIT conditions (3.18), they certainly lack the sense of *no signalling* due to the protocol implemented above [17].

We can then invoke the arguments of Fine's theorem given in the previous section. Inequalities (3.8) in the context of the LG framework becomes:

$$1 + s_i \langle Q_i \rangle + s_j \langle Q_j \rangle + s_i s_j C_{ij} \ge 0, \tag{3.25}$$

these are the twelve LG2s (2.32) given in section 2.5. Similarly, inequalities (3.14)-(3.17) now become the four LG3s (2.41)-(2.44). Fine's theorem guarantees the existence of an underlying probability distribution,  $p(s_1, s_2, s_3)$ , provided that the three sets of LG2s, compatibility conditions (3.20) and the set of LG3s are satisfied. Hence, the set of necessary and sufficient conditions for MR<sub>weak</sub> reads:

$$MR_{weak} = LG_{12} \wedge LG_{23} \wedge LG_{13} \wedge LG_{123} \wedge NIM_{pw} \wedge Induction, \qquad (3.26)$$

where  $LG_{ij}$  is the set of LG2s for measurements at times  $t = t_i$  and  $t = t_j$ , similarly  $LG_{123}$  is the set of LG3s, and  $\wedge$  denotes logical conjunction. Compared with the original LG framework, which involves obtaining the three correlation functions in three separate experiments to test the LG3s, this protocol consists of three additional experiments to obtain  $\langle Q_i \rangle$  and three more sets of LG2s to test. The set of inequalities with the LG2s and the LG3s combined are often referred to as the augmented set of LGIs, and they are the set of necessary and sufficient conditions for MR<sub>weak</sub> at three times.

This protocol can be readily extended to four times[17], and we find:

$$MR_{weak} = LG_{12} \land LG_{23} \land LG_{34} \land LG_{14} \land LG_{1234} \land NIM_{pw} \land Induction,$$
(3.27)

where  $LG_{1234}$  are the set of eight LG4s given by inequalities (2.33).

#### 3.2.2 Testing Macrorealism with NSIT

Under the assumption of NIM<sub>seq</sub>, a very different set of conditions can be derived for MR<sub>strong</sub> which do not involve the LGIs at all, see [38; 17; 39]. In this protocol, we assume a single experiment with sequential measurements at all three times is performed, from which we measure directly the joint probability,  $p_{123}(s_1, s_2, s_3)$ . Without assuming non-invasive measurements, we can write equation (3.3) as:

$$p_{123}(s_1, s_2, s_3) = \frac{1}{8} (1 + s_1 \langle Q_1 \rangle + s_2 \langle Q_2^{(1)} \rangle + s_3 \langle Q_3^{(12)} \rangle + s_1 s_2 C_{12} + s_2 s_3 C_{23}^{(1)} + s_1 s_3 C_{13}^{(2)} + s_1 s_2 s_3 D),$$
(3.28)

where the superscripts denote that the value of quantity depends on whether the measurement at times labelled by the superscript is performed. For example, the value of  $C_{23}^{(1)}$  depends on whether the measurement at  $t = t_1$  is performed, and  $\langle Q_3^{(12)} \rangle$  depends on whether both measurements at the two earlier times are performed. Note here we only included earlier or intermediate measurements in the superscript, but not later measurements. This is because induction is assumed throughout, also called the "arrow of time" in the paper by Clemente and Kofler[38].

Equation (3.24) is a measured probability that is non-negative by definition, but it is not the underlying joint probability distribution we seek since MR requires a joint probability such that there can be no dependence on which measurements are actually performed. As we will see below, by imposing a set of NSIT conditions, we can ensure that equation (3.24) becomes the same as the probability of an independent set of variables,  $Q_i$ .

We will begin the proof with a more rigorous definition of the NSIT condition:

NSIT<sub>(i)j</sub>: 
$$p_j(Q_j) = p_{ij}(Q_j) = \sum_{s_i} p_{ij}(s_i, s_j).$$
 (3.29)

As noted in [38], NSIT<sub>(2)3</sub> alone is a strong condition that can already detect violations of MR more reliably than the LG3s[40; 28]. However, it fails for certain initial states. This can be fixed by always performing measurements at  $t = t_1$ , and the resulting conditions are:

NSIT<sub>1(2)3</sub>: 
$$p_{13}(s_1, s_3) = p_{123}(s_1, s_3) = \sum_{s_2} p_{123}(s_1, s_2, s_3),$$
 (3.30)

and,

NSIT<sub>(1)23</sub>: 
$$p_{23}(s_2, s_3) = p_{123}(s_2, s_3) = \sum_{s_1} p_{123}(s_1, s_2, s_3).$$
 (3.31)

As a side note, Maroney and Timpson, in their paper, has proved that NSIT<sub>1(2)3</sub> and NSIT<sub>(1)23</sub> combined, along with the assumption of induction, are sufficient to imply the satisfaction of the LG3s[12], however, not MR. Referring back to equation (3.24), NSIT<sub>(1)23</sub> then implies that  $C_{23}^{(1)} = C_{23}$ ,  $\langle Q_2^{(1)} \rangle = \langle Q_2 \rangle$  and  $\langle Q_3^{(12)} \rangle = \langle Q_3^{(2)} \rangle$ . Similarly, NSIT<sub>1(2)3</sub> implies  $C_{13}^{(2)} = C_{13}$  and  $\langle Q_3^{(12)} \rangle = \langle Q_3^{(1)} \rangle$ , but the union of both conditions allows us to write  $\langle Q_3^{(12)} \rangle = \langle Q_3^{(1)} \rangle = \langle Q_3^{(2)} \rangle$ . Finally, we can impose NSIT<sub>(2)3</sub>, which then implies  $\langle Q_3^{(12)} \rangle = \langle Q_3^{(1)} \rangle = \langle Q_3^{(2)} \rangle = \langle Q_3 \rangle$ . Therefore, under these three assumptions, we find that all the superscripts in equation (3.24) are removed, and we end up with a joint probability distribution that satisfies all the requirements of MR. To be explicit, we have found the set of necessary and sufficient conditions for MR:

$$MR_{strong} = NSIT_{(2)3} \land NSIT_{(1)23} \land NSIT_{1(2)3} \land induction.$$
(3.32)

To summarize, we have now found the sets of necessary and sufficient conditions for both versions of macrorealism. The notion of the "strength" of MR comes from the fact that, for reasons to become apparent in the next section,  $MR_{strong}$  implies  $MR_{weak}$ , but not the other way around. In the augmented LG framework, we assume that NIM is satisfied by how we implement the measurements, and we set out to test the existence of *an* underlying probability distribution that is compatible with MR. Whereas in the NSIT formulation, we measure a three-time probability and impose a set of NSIT conditions, which, if satisfied, we obtain *the* underlying probability distribution that is compatible with MR. In this way, we can view the set of NSIT conditions as tests of NIM<sub>seq</sub>, which, if satisfied, immediately implies MRps and then MR[38], since NIM<sub>seq</sub> allows us to measure the system with arbitrarily small time intervals and as many times as we desire. We also note the apparent but significant fact that the set of NSIT conditions are equalities rather than inequalities as compared to the augmented LG framework. This goes to show that the conditions for MR<sub>strong</sub> are far more restrictive than the ones for MR<sub>weak</sub>.

The two protocols described above clearly investigate the two extremes of interpretations of MR, depending on how strongly NIM is assumed. There is, in fact, a hierarchy of MR which can be tested depending on the protocol. As Halliwell proposed in his paper, an intermediate (int) version of MR can be defined[17], of which the set of necessary and sufficient conditions are,

$$MR_{int} = NSIT_{(1)2} \land NSIT_{(2)3} \land NSIT_{(1)3} \land LG_{123} \land Induction,$$
(3.33)

a mixture of two-time NSIT conditions and the LG3s.

### 3.3 Quantum-Mechanical Analysis

#### 3.3.1 Quasi-Probability

Consider a system with Hamiltonian  $\hat{H}$ , measurements of the dichotomic variable Q on the system at time t can be written as the projection operator,  $\hat{P}_s(t) = e^{i\hat{H}t}\hat{P}_s e^{-i\hat{H}t}$ , where  $\hat{P}_s$  is given by:

$$\hat{P}_s = \frac{1}{2} \left( 1 + s\hat{Q} \right), \tag{3.34}$$

here we note that the projection operators,  $\hat{P}_s$  and therefore  $\hat{P}_s(t)$ , sum to 1. The probability,  $p_{ij}(s_i, s_j)$ , of two sequential projective measurements, according to the Born rule, is then given by:

$$p_{ij}(s_i, s_j) = \text{Tr}(P_{s_i}(t_j) P_{s_i}(t_i) \rho P_{s_i}(t_i)),$$
(3.35)

where  $\rho$  is the reduced density operator of the system, and we have dropped the hats on the operators for simplicity. By contrast, the two-time probabilities given by equation (3.23) in quantum mechanics correspond to the quasi-probabilities:

$$q(s_i, s_j) = \frac{1}{2} \operatorname{Tr}[(P_{s_i}(t_i) P_{s_j}(t_j) + P_{s_j}(t_j) P_{s_i}(t_i))\rho],$$
(3.36)

where again, we assume that it is calculated from the results of separate experiments. Equation (3.36) is real and sums to 1, but it can be negative at times, therefore, it is not a probability in general. We see here that the quasi-probabilities are clearly related to the set of LG2s in the augmented LG framework since they both originate from equation (3.23). Furthermore, if we impose the LG2s, this requires that  $q(s_i, s_j) \ge 0$ .

When we sum over the two measurements in equation (3.35), we find:

$$\sum_{s_j=\pm 1} p_{ij}(s_i, s_j) = \operatorname{Tr}(P_{s_i}(t_i)\rho P_{s_i}(t_i)) = \operatorname{Tr}(P_{s_i}(t_i)\rho) \equiv p_i(s_i),$$
(3.37)

when we sum over the second measurement, and,

$$\sum_{s_i=\pm 1} p_{ij}(s_i, s_j) = \text{Tr}(P_{s_j} \rho_M(t_i)),$$
(3.38)

where we sum over the first measurement and  $\rho_M$  denotes the measured density operator,

$$\rho_M(t_i) = \sum_{s_i = \pm 1} P_{s_i}(t_i) \rho P_{s_i}(t_i).$$
(3.39)

We note that equation (3.38) does not equal to the single time probability,  $p_j(s_j) = \text{Tr}(P_{s_j}(t_j)\rho)$ , in general. Therefore, we can immediately conclude that the two-time NSIT conditions (3.29) are not satisfied in quantum mechanics in general.

When we perform the same calculations on the quasi-probabilities of equation (3.36), however, we find that:

$$\sum_{s_j=\pm 1} q(s_i, s_j) = \frac{1}{2} (2P_{s_i}\rho) = p(s_i),$$
(3.40)

$$\sum_{s_i=\pm 1} q(s_i, s_j) = \frac{1}{2} (2P_{s_j}\rho) = p(s_j).$$
(3.41)

This is the exact same situation as the case with equation (3.24) in that the quasiprobabilities satisfy the set of conditions that is mathematically equivalent to the NSIT conditions since they are linear in both projection operators. Conditions of the form (3.40) and (3.41) are sometimes referred to as the *generalized no-signaling in time* conditions.

The relation between the probabilities and quasi-probabilities is given by:

$$q(s_i, s_j) = p_{ij}(s_i, s_j) + \frac{1}{8} s_j \left\langle [\hat{Q}(t_j), \hat{Q}(t_i)] \hat{Q}(t_i) \right\rangle,$$
(3.42)

where the extra term on the RHS of the equation is a measure of interference between two non-commuting measurements.

We see that if the interference term vanishes, then  $p_{ij}(s_i, s_j) = q(s_i, s_j)$ , and the two-time NSIT conditions (3.29) are satisfied exactly. Additionally, by imposing the two-time NSIT conditions, we see that this immediately implies  $q(s_i, s_j) \ge 0$ , which is equivalent to the satisfaction of the LG2s. However, this relation clearly does not work in reverse; by imposing the LG2s, it only requires that the interference term is bounded by:

$$\frac{1}{8} \left| \left\langle [\hat{Q}(t_i), \hat{Q}(t_j)] \hat{Q}(t_i) \right\rangle \right| \le p_{ij}(s_i, s_j).$$
(3.43)

Even though we have only considered the measurement at two-times, the same conclusion can be drawn in the general case, where we see that MR<sub>strong</sub> involving the NSIT conditions requires zero interference but MR<sub>weak</sub>, which makes use of the LGIs, only requires bounded interference. Hence, we have shown that, from a quantum-mechanical viewpoint,

$$MR_{strong} \Rightarrow MR_{weak}.$$
 (3.44)

Note that at two times, the NSIT condition (3.29) and the LG2s (3.26), i.e.,  $q(s_1, s_2) \ge 0$ , are both necessary and sufficient conditions for MR, but a violation means different things. As stressed many times before, when measuring  $q(s_1, s_2)$ , NIM is assumed by the measurement scheme. Therefore, in an *ideal* situation, the LG2s can be considered as a direct measure of MRps directly. However, there is always the clumsiness loophole which arguably cannot be avoided. In contrast, the NSIT conditions are different in the sense that it is thought of as testing a combination of both NIM and MRps, and we are unable to distinguish between them.

#### 3.3.2 Quantum Witness

In the two-time case, we can quantify the invasiveness of the first measurement by defining a quantum witness:

$$W(s_2) = \left| p_2(s_2) - \sum_{s_1} p_{12}(s_1, s_2) \right|, \qquad (3.45)$$

which is the difference between the probabilities, of obtaining,  $s_2$  if we measured it directly and that given by equation (3.38). These familiar looking-terms are of course closely related to the NSIT conditions, and the witness can then be thought of as a measure of the degree to which NSIT is violated in the familiar qubit-like system, which consists of a single dichotomic variable Q. However, equation (3.45) is very general in that it imposes no restrictions on the particular set-up, e.g., the variables of the first and second measurements can be different, and they can both be many-valued.

The value of  $W(s_2)$  is clearly bounded between 0 and 1, for which a value of 0 corresponds to classical behaviour. It is proved that for a general *N*-level system, the maximum value of  $W(s_2)$  is given by[41]:

$$W^{max}(s_2) = 1 - \frac{1}{N},$$
 (3.46)

which permits a bigger violation of the LGIs that exceeds the limit in the two-level case, which we will discuss in more detail in the following sections.

If the first measurement is indeed non-invasive, we should then expect that:

$$W = 0, \tag{3.47}$$

this is known as the quantum-witness equality [41].

Returning to the discussion on a qubit-like system, it can be shown that this witness, in fact, is proportional to the interference term[17],

$$W(s_2) = \frac{1}{4} \left| \left\langle [\hat{Q}(t_j), \hat{Q}(t_i)] \hat{Q}(t_i) \right\rangle \right|.$$
(3.48)

Hence, the witness can also be used to check the LG2s, for which the condition is:

$$\frac{1}{2}W(s_2) \le p_{12}(s_1, s_2),\tag{3.49}$$

much similar to the inequalities (3.43).

### 3.4 Many-Valued Variables

The original proposed LG framework, and a part of the later developments in this area, is primarily focused on two-level systems with a single dichotomic variable Q, which is very restrictive on how we can test different systems. We note that variables, but it is actually the measurement outcomes that we deal with, being many-valued, can have different origins, and they can have different effects on the LGIs, depending on the dimension of the system, i.e., the number of states, N, and the type of measurements, i.e., weak or projective. There are a few cases to be considered.

We have already seen that when performing weak measurements on a dichotomic variable, Q, as discussed in section 2.6, the range values of the measurement outcome, q, exceeds the range of Q, and in turn, that of the outcomes of projective measurements, s, and q can even be continuous. In this case, q, being many-valued, can be easily incorporated into the LGIs by simply requiring that  $\langle Q \rangle = \langle q \rangle$ , this can be achieved by calibrating the detector, and as a result, we get LGIs similar to equation (2.56).

Another possibility is that the quantity we are interested in, of a system, is inherently multi-valued, for example, the spin of a spin- $\frac{3}{2}$  particle. A projective measurement on such a N-level system can project the state of a system onto one of Mdifferent subspaces. In general, we could also choose  $2 \le M \le N$ . We could choose M = 2, in which case, the LG framework remains unaffected, which admits the same patterns of violation as it would if N = 2[42]. For the  $2 < M \leq N$ , we can nevertheless choose to assign a value of  $Q = \pm 1$  to each outcome of the measurement, such that Q = +1 corresponds to a fraction of all possible measurement outcomes and Q = -1 corresponds to the rest. In this way, the LGIs remain the same; however, the maximum violation of the LGIs are found to be affected by both M and N[43], exceeding the value of  $\frac{3}{2}$  for the LG3s. In exploiting this interesting feature, the LGIs have been proposed to serve as a dimension witness [44], in providing a lower bound on the number of quantum levels an experimenter is able to manipulate[43], and also a possible connection to equation (3.46). However, reducing the measurement outcome in this way makes the test incomplete in that we have not considered all the possible ways to construct the dichotomic variable Q.

We can, however, adopt a complete approach in dealing with  $2 < M \leq N$  by rewriting the *M*-value outcomes as a *set* of *M* dichotomic variables, Q(n), for n = 1, ..., M, this is proposed by Halliwell et al.[39], this approach leads to a reformulation of the original LG framework, and the set of necessary and sufficient conditions for MR, in this case, are also found in the same paper. We will follow the formulation of Halliwell et al. and present some of their findings in the remainder of this section.

Consider a projective measurement with a set of M projection operators labelled by n,  $\hat{E}_n$ , such that:

$$\sum_{n} \hat{E}_{n} = \mathbb{1}, \qquad (3.50)$$

where we have used a different letter, E, to distinguish from the N = M = 2 case, i.e., equation (3.34). The most general dichotomic variable one can construct from the projectors has the form:

$$\hat{Q} = \sum_{n} \epsilon(n) \hat{E}_{n}, \qquad (3.51)$$

where  $\epsilon(n) = \pm 1$  and contains at least one of each. However, it is found to be sufficient to consider a subset of  $\hat{Q}$  whose  $\epsilon(n)$  only has a single +1, for the purpose of constructing the many-valued LG framework[39]. We can then label these  $\hat{Q}$  by n, and they can be written as:

$$\hat{Q}(n) = \hat{E}_n - \sum_{n' \neq n} \hat{E}_{n'} = \hat{E}_n - (\mathbb{1} - \hat{E}_n) \equiv \hat{E}_n - \hat{\bar{E}}_n, \qquad (3.52)$$

where  $\hat{E}_n$  corresponds to the negation of  $\hat{E}_n$ . We, therefore, obtain a formula similar to equation (3.34):

$$\hat{E}_n = \frac{1}{2}(\mathbb{1} + \hat{Q}(n)),$$
(3.53)

where we note the lack of a minus sign compared to equation (3.34), for reasons to become clear later.

From equation (3.50), we can find that the sum of  $\hat{Q}(n)$ :

$$\sum_{n} \hat{Q}(n) = (2 - M)\mathbb{1}.$$
(3.54)

This is a constraint that the set of  $\hat{Q}(n)$  must satisfy; hence, this is a non-minimum set, and there are only M - 1 independent variables in the system.

We are now ready to obtain the LGIs. We will start by denoting the classical counterparts to  $\hat{Q}(n)$  and  $\hat{E}(n)$  as  $Q_i(n_i)$  and  $E_i(n_i)$ , at time  $t = t_i$ . Here we note that the classical counterpart to the projection operators  $\hat{E}(n)$ , has values  $E_i(n_i) \in \{0, 1\}$ , such that  $E_i(n_i) = 1$  denotes that the system is projected onto the state  $|n_i\rangle$ . We can easily generalize equation (3.23) to the many-value case as:

$$p(n_1, n_2) = \langle E_1(n_1) E_2(n_2) \rangle = \frac{1}{4} (1 + \langle Q_1(n_1) \rangle + \langle Q_2(n_2) \rangle + \langle Q_1(n_1) Q_2(n_2) \rangle),$$
(3.55)

where we assume that the terms on the right are all measured in a non-invasive fashion, similar to before. We can immediately obtain the LG2s in the many-valued case by requiring that  $p(n_1, n_2) \ge 0$ :

$$1 + \langle Q_1(n_1) \rangle + \langle Q_2(n_2) \rangle + \langle Q_1(n_1)Q_2(n_2) \rangle \ge 0,$$
(3.56)

and there are a total of  $M^2$  inequalities. Exactly the same as the two-level case, these  $M^2$  LG2s are the necessary and sufficient conditions for the existence of the underlying joint probability,  $p(n_1, n_2)$ , i.e., it is non-negative, and hence, MR<sub>weak</sub>. Compared to the usual LG2s, apart from the obvious difference where the label  $s_i$ is replaced with  $n_i$ , it can be easily spotted that equation (3.56) contains no minus signs. This is a consequence of utilizing a non-minimum set, we can replace  $Q_i(n_i)$  with  $-Q_i(n'_i)$  since,

$$\sum_{n_i \neq n'_i} E_i(n_i) = 1 - E(n') = \bar{E}(n').$$
(3.57)

Therefore, the set of LG2s (3.56) is equivalent to any other set with any number of minus signs in it, and it is the same for equation (3.53). For a set-up where, M = 2, then we find  $Q_i(1) = -Q_i(2)$ , and we retrieve the usual two-level LG2s, as expected. Similarly, for M = 3, the dichotomic variables obey equation (3.54), and we have  $Q_i(1) + Q_i(2) + Q_i(3) = 1$ , which means we can replace  $Q_i(3)$  with  $1 - Q_i(1) - Q_i(2)$ . Writing them out explicitly, the LG2s for the case M = 3 are[39]:

$$1 + \langle Q_1 \rangle + \langle Q_2 \rangle + \langle Q_1 Q_2 \rangle \ge 0, \tag{3.58}$$

$$1 + \langle R_1 \rangle + \langle Q_2 \rangle + \langle R_1 Q_2 \rangle \ge 0, \tag{3.59}$$

$$1 + \langle Q_1 \rangle + \langle R_2 \rangle + \langle Q_1 R_2 \rangle \ge 0, \tag{3.60}$$

$$1 + \langle R_1 \rangle + \langle R_2 \rangle + \langle R_1 R_2 \rangle \ge 0, \tag{3.61}$$

$$\langle Q_1 \rangle + \langle R_1 \rangle + \langle Q_1 Q_2 \rangle + \langle R_1 Q_2 \rangle \le 0,$$
 (3.62)

$$\langle Q_1 \rangle + \langle R_1 \rangle + \langle Q_1 R_2 \rangle + \langle R_1 R_2 \rangle \le 0$$
(3.63)

$$\langle Q_2 \rangle + \langle R_2 \rangle + \langle Q_1 Q_2 \rangle + \langle Q_1 R_2 \rangle \le 0, \tag{3.64}$$

$$\langle Q_2 \rangle + \langle R_2 \rangle + \langle R_1 Q_2 \rangle + \langle R_1 R_2 \rangle \le 0, \tag{3.65}$$

$$\langle Q_1 Q_2 \rangle + \langle Q_1 R_2 \rangle + \langle R_1 Q_2 \rangle + \langle R_1 R_2 \rangle \ge 0, \tag{3.66}$$

where we have adopted the notation  $Q_i \equiv Q_i(1)$  and  $R_i \equiv Q_i(2)$ . The ability to write the LG2s in this form is clearly beneficial in an experimental setting since one of the M states needs not to be measured. This also reflects the fact that there are only M - 1 free variables in this framework.

Higher order LGIs can be found in a similar fashion as above, and combined with Fine's theorem described in earlier sections, we can easily prove that the set of necessary and sufficient conditions for MR<sub>weak</sub> have the exact same form, but with the newly found many-valued LGIs. In general,  $n^{th}$ -order LGIs will consist of  $M^n$  inequalities, consistent with the M = 2 results we have found before.

We can also consider NSIT conditions for  $MR_{strong}$  in the many-valued case. It is found that at two times, there are  $\frac{M(M-1)^2}{2}$  different ways interference can occur, each represented by an interference term that needs to be fixed to zero to ensure  $MR_{strong}$ [39]. There are, in general, M - 1 independent two-time NSIT conditions of the form:

$$p_2(n_2) - \sum_{n_1=1}^{N} p_{12}(n_1, n_2) = 0.$$
 (3.67)

Additionally, it is also completely natural to require that:

$$p_2(n_2) - \sum_{s_1} p_{12}^{Q_1(n_1)}(s_1, n_2) = 0, \qquad (3.68)$$

where  $p_{12}^{Q_1(n_1)}\left(s_1,n_2\right)$  is obtained by measuring one of the dichotomic variable  $Q_1(n_1)$ as the first measurement. It can be shown that the NSIT conditions in equation (3.68) each tests a different mixture of interference terms; therefore, they count as further independent conditions to equation (3.67). Unlike equation (3.67), however, the number of independent conditions of the form (3.68) depends on the number of different dichotomic variables we are considering. For a set of M' Q(n), and M' = M, like the one we have been using in the LG case, there will be a total of (M-1)M independent NSIT conditions. The total number of independent NSIT conditions we can derive from M dichotomic variables is then (M + 1)(M - 1), for  $M \geq 3$ . For M = 3, we can find  $4 \times 2 = 8$  two-time NSIT conditions, but only  $\frac{3(3-\overline{1})^2}{2} = 6$  of them are needed to ensure that interference is zero. For M = 4, and in general M > 4, we find that the number of independent two-time NSIT conditions is less than the number of interference terms that need fixing. In order to find a full set of NSIT conditions suitable for MR<sub>strong</sub>, we would need to consider more dichotomic variables of the form given by equation (3.51). In summary, then, the set of Q(n) is enough to find all the LGIs we need for MR<sub>weak</sub>, we need to consider the set of all possible dichotomic variables to find sufficiently many NSIT conditions to ensure MR<sub>strong</sub>. This also reflects the fact that MR<sub>strong</sub> is a much stricter notion than MR<sub>weak</sub>, as we have discussed in previous sections.

#### 3.5 Macrorealism per se

As Peres noted in his paper[45], realism has "as least as many definitions as there are authors". It is criticized that the original wording of the MRps statement is ambiguous. At first glance, MRps implies two things, that the system is in a definite state at all times and that no linear superpositions of *macroscopically distinct states* are allowed for a macroscopic system. The first is consistent with the notion of *realism* we have been discussing so far, and we can immediately draw the conclusion that there exists an underlying joint probability distribution in the same way as the Bell/CHSH case. Regarding the denial of superposition and the exact meaning of the words "macroscopically distinct states", however, the exact interpretation and the validity of this statement have been debated by many authors[12; 46].

We have already seen how the different interpretations of the NIM condition can lead to different versions of MR; however, as we will discuss in this section, different interpretations of the MRps condition can also lead to different versions of MR, as argued by Maroney and Timpson in their 2014 paper[12]. By carefully considering the preparation stage of each experiment and the resulting state the system is in, we are able to find different interpretations of MRps. Specifically, the authors have identified three different varieties of MRps, namely:

- 1. Operational eigenstate mixture macrorealism,
- 2. Operational eigenstate support macrorealism,
- 3. Supra eigenstate support macrorealism.

To properly define these different assumptions and understand the differences, we need to consider a couple of definitions first. An operational eigenstate of a macroscopic physical quantity Q is defined such that a measurement of Q on such a state will return a particular value  $q_i$  with certainty, i.e.,  $p(Q = q_i) = 1$ . We can also assume that immediately after a measurement, the system will be in the corresponding operational eigenstate, such that if we perform a second measurement immediately following the first, we will find the same result. Note that an operational eigenstate is defined in a macroscopic way and need not to be in a one-to-one correspondence with the ontic states. In this way, if the system is in an operational eigenstate before the measurements, and we have checked that the type of measurement, when performed on such operational eigenstates, does not affect the subsequent evolution of the system, we can then assume that the NIM condition holds. The second definition is that of the support: given a quantum system with (microscopic) states,  $\lambda \in \Lambda$ , where  $\Lambda$  is the set of all possible quantum states, an arbitrary state of the system can be described with a probability distribution over  $\lambda$ , denoted as  $\mu(\lambda)$ , and the corresponding support of that state is defined as:

$$\operatorname{supp}(\mu) \equiv \{\lambda | \mu(\lambda) > 0\}, \tag{3.69}$$

i.e., the set of states  $\lambda$  which  $\mu(\lambda) > 0$ .

The notion of *realism* requires that every possible quantum state  $\lambda \in \Lambda$  is macrodefinite for Q. It is then also natural to assume that every quantum state can be accessed by one of the operational eigenstates. Even though a general preparation procedure can result in a non-macrodefinite state, but it is nothing more than a statistical mixture of operational eigenstates due to our ignorance of the preparation procedure. This view is called the operational eigenstate mixture macrorealism. It assumes that the distribution of a general state  $\mu(\lambda)$  can always be written as:

$$\mu(\lambda) = \sum_{i} a_{i} \mu_{q_{i}}(\lambda), \qquad (3.70)$$

where  $\mu_{q_i}(\lambda)$  can be written as a convex sum of that of operational eigenstates such that every state in  $\text{supp}(\mu_{q_i})$  is value-definite with  $Q = q_i$ , and  $a_i \ge 0$ , appropriately valued such that  $\mu(\lambda)$  is normalized. Clearly, under this version of MRps, NIM can hold at all times, and a violation of the LGIs implies a violation of MRps.

By contrast, operational eigenstate support macrorealism assumes a more general version of equation (3.70):

$$\mu(\lambda) = \sum_{i} a_i \nu_{q_i}(\lambda), \qquad (3.71)$$

where  $\nu_{q_i}(\lambda) > 0$  only if  $\lambda$  can be accessed by the corresponding  $q_i$  operational eigenstate, and can be negative in general. The difference compared to the operational eigenstate mixture macrorealism is that the quantity  $\nu_{q_i}(\lambda)$  cannot be obtained from a statistical mixture of operational eigenstates in general. In this way, even though a measurement has been tested thoroughly to be non-invasive for operational eigenstates, it may still turn out to be invasive for a general state. An example of theories matching this description is the Kochen-Specker model[47].

Lastly, if we lift the assumption that every macrodefinite state  $\lambda$  can be accessed by one of the operational eigenstates, we arrive at the last variety: supra eigenstate support macrorealism. More specifically, there exist states which can be accessed only when the system is in a mixture of two or more operational eigenstates. The probability distribution  $\mu(\lambda)$  is still given by equation (3.71), but we assume that  $\nu(\lambda)$  can be bigger than zero, even if  $\lambda$  cannot be accessed by the  $q_i$  operational eigenstate. An example of such theories is the de Broglie-Bohm theory, also known as the pilot wave interpretation of quantum mechanics.

The validity of these assumptions can be found in the original paper[12]. The crucial point here is that even though all three cases admit realism about the macroscopic, that for all  $\lambda \in \Lambda$  is macrodefinite, only the first case of MRps can be definitively ruled out by a violation of the LGIs, whereas a violation in the remaining two cases can both be considered as a violation of NIM, rather than MRps. This is consistent with our discussion on the clumsiness loophole in the previous sections, that in theories like the de Broglie-Bohm interpretation, the last two kinds of MRps cannot be ruled out definitively by the LG framework. However, as noted by the author, both kinds are not particularly welcome since they seem to suggest quantum behaviours at a macroscopic level.

## 3.6 Summary

This chapter is focused mainly on finding the set of necessary and sufficient conditions for macrorealism, motivated mainly by Fine's theorem in Bell's case. We have shown that Fine's theorem can be applied to the LG framework, provided we specify the measurement protocol or a set of two-time NSIT-like compatibility conditions as equation (3.24) holds. When extending to more measurement times and higherdimensional systems, the generalized Fine's theorem allows us to find the sets of necessary and sufficient conditions for both cases.

In searching for necessary and sufficient conditions for MR, we must inevitably consider all the interpretations of MR. As we have briefly shown in this chapter, the exact interpretation of both the NIM and MRps assumptions can have an impact on the exact definition of MR and how we test for it. Notably, we can obtain a hierarchy of different MR, depending on how strongly we implement the NIM conditions in our experiments. On the one hand, we can require that the only first measurement of the pair of sequential measurements is non-invasive, and that we perform at most two measurements in an experiment, i.e., NIM<sub>pw</sub>. The corresponding MR is denoted MRweak, and we find that the set of all possible LG2s and LG3s is sufficient to prove MR<sub>weak</sub> at *n*-time, as indicated by the generalized Fine ansatz (3.21). On the other hand, by requiring that any number of sequential measurements can be non-invasive, we obtain MR<sub>strong</sub>. The assumption of NIM<sub>seq</sub> is checked by NSIT conditions, when combined appropriately, they form a set of necessary and sufficient conditions for MR<sub>strong</sub>. We have also seen explicitly that, in the quantum-mechanical formulation, both notions of MR pose restrictions on the amount of interference between measurements, and the LG framework only requires that interference is sufficiently small. An important point to note is that we must consider a set of NSIT conditions that is sufficiently large compared to the possible interference terms before concluding anything regarding MR. For example, in the many-value case, as we have seen in section 3.4, special care must be taken with the set of dichotomic variables we use in order to obtain enough NSIT conditions to kill interference completely, only then can we begin to test for MR<sub>strong</sub>.

In the last section, we have briefly discussed different interpretations of the MRps. These are specified through the distinction between the operational eigenstates and the true state of the system, which, in the case of quantum mechanics, are the quantum states themselves. The paper by Maroney and Timpson, considered by most readers a blunt criticism of the LG framework, defined the three varieties of MRps and proved that the LGIs are only useful for ruling out one of them. This feature is, of course, closely related to the clumsiness loophole. There is seemingly no way to prove a measurement is non-invasive once and for all, at least not by testing it experimentally since there always exist some other tests which are not yet performed. Therefore, we can never fully close the clumsiness loophole, which, in turn, would give us hope of falsifying MRps. There are many proposals in wishing to address the clumsiness loophole, including the continuous in time velocity measurements like we have discussed, see also Ref. [23; 48], but such a loophole remains to date.

## Chapter 4

## **Related Works and Overview**

As we have already seen in the previous sections, the LG framework can be adapted to various forms depending on the experimental set-up. In general, the experiments all involve testing the system against selective sets of inequalities involving time correlation functions, similar to the original LGIs. We have included a few examples of what they could look like in sections 2.5, 2.6 and 3.4.

Particularly, we have not yet discussed the pentagon inequality (PI), equation (2.45). In the paper by Majidy et al.[49], a numerical simulation is performed, and they have found that there exist regimes where the PI is violated while satisfying all the corresponding LG2s and LG3s. This is consistent with the fact that the PI is irreducible, that it can not be obtained from combining the LG3s. In general, we can define n-gon inequalities[37]:

$$n+2\sum_{i< j} s_i s_j C_{ij} \ge \begin{cases} 1 & \text{if } n \text{ odd,} \\ 0 & \text{if } n \text{ even,} \end{cases}$$
(4.1)

and it is found that the set of all possible LG2s, LG3s and the *n*-gon inequality are the necessary and sufficient conditions for MR at *n*-time. Compared to the original *n*-time LG framework, testing the *n*-gon inequalities requires more measurements to be taken, e.g., all possible two-time correlation functions. More measurements lead to more potential interference terms, and hence the set of sufficient conditions varies, as expected. Here we note that we could also extend our measurement scheme to include higher-order correlation functions, this is discussed in [50].

Another interesting form of LGIs is derived in a paper by Emary [48] when considering ambiguous measurements, the classical analogue of weak experiments. In which, the author is able to derive a set of LGIs without invoking the NIM assumption, which takes into account the invasiveness of the measurements, by adding a term to the LGIs similar to the quantum witness given by equation (3.45). Such LGIs cannot be violated in experiments, following similar reasoning to that of inequality (2.18). However, by performing ambiguous measurements instead of unambiguous ones, together with the assumption "equivalently invasive measurability" (EIM), which states that ambiguous measurements are equally invasive as non-ambiguous ones, violations of LGIs can be detected. By tailoring the experimental set-up to best satisfy EIM, a violation would force a macrorealist to either reject MRps or find reasons to explain how two types of measurements can collude to give the same amount of signalling and yet affect the system in drastically different ways[48]. In this case, the clumsiness loophole clearly does not apply, but it is replaced with a "collusion loophole", which is arguably smaller. We note here that this is of a similar methodology to the test proposed in [23], and carried out experimentally in [51].

The LG framework can also be adapted into testing interference experiments, where macroscopic coherence, arguably, is already observed [52; 53; 54; 55]. As Pan noted in his paper, there are no measurements taken during each experiment hence NIM essentially plays no role in violating the LGIs. A detailed analysis found that violations of LGIs are always accompanied by destructive interference[52], and, of the same origin, anomalous weak values[53]. In this case, situations where the LGIs are satisfied simply imply that the level of interference in the system is sufficiently small, that we can essentially treat the system as classical, and, in principle, assign probabilities to the object passing each slit. Similar experiments are also performed with a triple-slit set-up and simple harmonic oscillators, and the regimes where the LGIs are violated are identified.

LGIs can also function as a coherence witness in studying open systems, the behaviour of the LGIs in such systems is also studied[56; 57; 11; 58], however, as noted by Wang et al.[59], the degree of violation cannot be taken directly as a measure of quantumness. Nevertheless, the LGIs are still very useful in studying the effect of dephasing on quantum systems, and this is particularly important in testing quantum hardware such as quantum computers[60; 61].

In summary, we have seen various examples of the capabilities of the LG framework. Despite the fact that it fails to rule out a particular natural class of theories, unlike Bell's inequalities, the LG framework has many applications in studying quantum systems from a whole new perspective. However, it does not come without challenges, namely, the assumption that a measurement can be non-invasive is inherently incompatible with quantum mechanics. This makes it difficult to interpret a violation and distinguishing between the corresponding assumption or assumptions that have been shown to be false. A macrorealist will always use the clumsiness loophole to try to protect MRps, and future experiments need to present far more convincing arguments to change that. Potential future work in this subject includes extending the framework to larger systems, finding more refined measurement protocols, studying the effect of noise on the system and, ultimately, understanding when and how classical behaviour emerges from quantum mechanics.

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