Violation of a Leggett-Garg inequality with ideal non-invasive measurements

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SUPPLEMENTARY INFORMATION

SUPPLEMENTARY METHODS

Constraints on macrorealism

Recall that each of the three core experiments are resolved into a further two sub-experiments, making six experiments in all. A macrorealist, under the assumption of non-invasive measurability, will concede that in the six experiments (which are performed on an identical initial state, and under the same conditions governing dynamics, i.e. the same Hamiltonian), the combined and post-selected results will be entirely equivalent to the family of three core experiments, each pair of circuits being equivalent to a single member of that family. Failure to post-select the results of measurements (as in e.g Ref.[22]) severely weakens the argument, and effectively introduces an extra assumption, namely that CNOT gates are always non-invasive. With proper post-selection then, the constraints (derived below) that are manifested in the Leggett-Garg inequality apply equally to the combined and post-selected results of the six lab experiments as they do to a single ideal experiment. This argument makes use of an additional assumption named 'Induction'. This is an assumption about the behaviour of identically prepared and identically treated ensembles, and essentially states that causality only runs forwards in time[23]. We take this assumption as self evident and so do not state it explicitly in the main paper. Furthermore we believe that this assumption is equally required by experiments utilising a spatial ensemble and those using a time ensemble.

All macrorealist theories are required to predict measurement statistics for the correlators involved in the Leggett-Garg inequality. The underlying theory of macrorealism, if it is to be consistent, must abide by the conservation of probability and other consistency conditions. For example consider a general macrorealist theory assigning probabilities $\mathbb{P}(\updownarrow_1\updownarrow_2\updownarrow_3)$ to each possible evolution of the system:

t_1	t_2	t_3	$\mathbb{P}$	f_{LG}
$\uparrow$	$\uparrow$	$\uparrow$	$\mathbb{P}(\uparrow_1\uparrow_2\uparrow_3)$	4
$\uparrow$	$\uparrow$	$\downarrow$	$\mathbb{P}(\uparrow_1\uparrow_2\downarrow_3)$	0
$\uparrow$	$\downarrow$	$\uparrow$	$\mathbb{P}(\uparrow_1\downarrow_2\uparrow_3)$	0
$\uparrow$	$\downarrow$	$\downarrow$	$\mathbb{P}(\uparrow_1\downarrow_2\downarrow_3)$	0
$\downarrow$	$\uparrow$	$\uparrow$	$\mathbb{P}(\downarrow_1\uparrow_2\uparrow_3)$	0
$\downarrow$	$\downarrow$	$\downarrow$	$\mathbb{P}(\downarrow_1\downarrow_2\downarrow_3)$	0
$\downarrow$	$\downarrow$	$\uparrow$	$\mathbb{P}(\downarrow_1\downarrow_2\uparrow_3)$	0
$\downarrow$	$\downarrow$	$\downarrow$	$\mathbb{P}(\downarrow_1\downarrow_2\downarrow_3)$	4

For consistency we have

$$\sum_{\updownarrow_1}\sum_{\updownarrow_2}\sum_{\updownarrow_3}\mathbb{P}(\updownarrow_1\updownarrow_2\updownarrow_3) = 1,$$

and for example

$$\mathbb{P}(\uparrow_1\downarrow_3) = \mathbb{P}(\uparrow_1\uparrow_2\downarrow_3) + \mathbb{P}(\uparrow_1\downarrow_2\downarrow_3).$$

Using these conditions each correlator may be calculated from the macrorealist table by choosing the two appropriate rows for each two-time correlator (tracing out the column for whichever time is not needed), i.e. :

t_1	t_2	$\mathbb{P}$	$Q(t_1)Q(t_2)$
$\downarrow$	$\downarrow$	$\mathbb{P}(\downarrow_1\downarrow_2\uparrow_3)$+$\mathbb{P}(\downarrow_1\downarrow_2\downarrow_3)$	1
$\downarrow$	$\uparrow$	$\mathbb{P}(\downarrow_1\uparrow_2\uparrow_3)$+$\mathbb{P}(\downarrow_1\uparrow_2\downarrow_3)$	-1
$\uparrow$	$\downarrow$	$\mathbb{P}(\uparrow_1\downarrow_2\uparrow_3)$+$\mathbb{P}(\uparrow_1\downarrow_2\downarrow_3)$	-1
$\uparrow$	$\uparrow$	$\mathbb{P}(\uparrow_1\uparrow_2\uparrow_3)$+$\mathbb{P}(\uparrow_1\uparrow_2\downarrow_3)$	1

One then multiplies each pairwise sum of probabilities by ± 1 according to whether that row was a correlation or anti-correlation. The lower bound for the Leggett-Garg inequality arises from the frustration of a given state being anti-correlated with at most one of the other states (but not both), and the fact that because no single evolution of the system can violate the inequality, no statistical sampling will.

An experimenter extracts correlations in the following way, with populations labelled $|\text{system}\rangle|\text{ancilla}\rangle$:

t_i	t_j	Population	Non Invasive?	Correlation?
$\downarrow$	$\downarrow$	$\lvert\downarrow\downarrow\rangle$	CNOT	+
$\downarrow$	$\uparrow$	$\lvert\uparrow\downarrow\rangle$	CNOT	-
$\uparrow$	$\downarrow$	$\lvert\downarrow\downarrow\rangle$	anti-CNOT	-
$\uparrow$	$\uparrow$	$\lvert\uparrow\downarrow\rangle$	anti-CNOT	+

Each of the classical trajectories can be probed non-invasively, by post-selecting populations from the appropriate circuit.

The stationarity assumption

Although others have used it (sometimes implicitly), the additional assumption of stationarity is first given explicitly by Huelga et al.[24]:

> "...the evolution from t_1 to t_2 is governed by the same stochastic differential equation as the evolution from t_2 to t_3, and this implies stationarity; that is $K(t_1, t_2) = K(t_1 - t_2)$".

This assumption is often used to redefine the Leggett-Garg Inequality

$$f = K(\tau) + K(2\tau) \geq -1 \tag{S1}$$

or similar. We note that there exist numerous macrorealist theories (which make predictions by distributing probability in the way outlined above) which are capable of violating (S1). Consider a macrorealist theory which has θ as it's hidden variable, and flips from one of it's states to the other with a probability proportional to the cosine squared of this angle. Such a theory is clearly capable of predicting Rabi oscillations. We take it to be an important feature of the original Leggett-Garg inequality that it is not violated by such theories.

Reducing the venality through hyperpolarisation

The unitary nuclear rotation U may be performed in a manner which is conditional on the system being in the 'correct' ancilla state $\downarrow$ because the postselected data will always correspond to the unitary operation U having been applied. If the rotation is conditional in this way, one of the two 'bad' populations becomes inactive and will not experience any evolution whatsoever in the course of the protocol (specifically state $|\downarrow\uparrow\rangle$ for the CNOT circuits and $|\uparrow\uparrow\rangle$ for the anti-CNOT circuits). The inactive state does not participate in the experiment and may be ignored. By minimising the population of the *single* active bad population we can reach a reduced effective venality. If the population distribution of all four energy levels is the same for the initial state of both circuits in each pair we have e.g. in the $\{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$ basis

$$\rho_C = \rho_A = \frac{1}{Z}\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & c & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & d \end{pmatrix}$$

where ρ_C and ρ_A are initial states prepared for CNOT and anti-CNOT circuits respectively, and $Z = a+b+c+d$ in both cases. The following expressions describe the lower bounds on quantum mechanical (QM), Moderate macrorealist (MMR) and Adversarial macrorealist (AMR) predictions:

$$\begin{aligned} g_{QM} &\geq \frac{1}{Z}(a+b-c-d)(\cos 2\theta + 2\cos\theta) \\ g_{MMR} &\geq -\frac{1}{Z}(a+b) \\ g_{AMR} &\geq -\frac{1}{Z}(a+b+3c+3d) \end{aligned}$$

where $g = K_{12} + K_{13} + K_{23}$ and $f = g + 1$. The venality $\zeta = (c+d)/Z$ allows one to write

$$g_{QM} \geq \ (1-2\zeta)(\cos 2\theta + 2\cos\theta) \tag{S2}$$
$$g_{MMR} \geq -(1-\zeta) \tag{S3}$$
$$g_{AMR} \geq -(1-\zeta) - 3\zeta. \tag{S4}$$

In thermal equilibrium $(a,b,c,d) = (1,\alpha,1,\alpha)$ and so in general $\zeta = 2\alpha/(2+2\alpha)$. When oscillations are only driven on those primary systems which were paired with a correctly initialised ancilla, one (system,ancilla) state always remains unused throughout the experiment. We exploit this fact by hyperpolarising the system so that the remaining active state has a lower population than is possible in thermal equilibrium at a given temperature. If the population distribution is identical across only the three active levels of the experiment we have

$$\rho_C = \frac{1}{Z}\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & [c] & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & d \end{pmatrix}$$

for the CNOT circuit and

$$\rho_A = \frac{1}{Z}\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & d & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & [c] \end{pmatrix}$$

for the anti-CNOT circuit with $Z = a + b + c + d$ as usual. The inactive state is denoted with [ ]. These different initial states, although physically distinct, are logically identical because the relevant active energy levels have the same population distribution. The predictions are now

$$g_{QM} \geq \ \frac{1}{Z}(a+b-2d)(\cos 2\theta + 2\cos\theta)$$
$$g_{MMR} \geq -\frac{1}{Z}(a+b)$$
$$g_{AMR} \geq -\frac{1}{Z}(a+b+6d).$$

Note that all predictions are independent of the inactive state with population c, except for in the normalisation Z. The normalisation can be arbitrarily scaled without affecting the comparison of the three predictions for g (or for f) since they will all be affected linearly in the same fashion. We choose to multiply g by $Z/(a+b+2d)$ so that there is a normalisation of $a+b+2d = Z_r$ and no longer any dependence on c. This allows us to define the venality as $\zeta = 2d/Z_r$ and to recover equations (S2),(S3),(S4). This technique is equivalent to supplying the single four level population distribution

$$\rho' = \frac{1}{Z_r}\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & d & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & d \end{pmatrix}$$

to both types of circuit. Using hyperpolarisation we achieve $(a,b,c,d) = (1,\alpha,\alpha,\alpha^2)$ so that $\zeta = 2\alpha^2/(1+\alpha+2\alpha^2)$.

Effect of detuned pulses

In the ideal scenario, the experimenter applies either the CNOT or anti-CNOT to the primary system-ancilla pair to perform the non-invasive measurement. In real spin resonance experiments each of the pulses will excite finite amplitude in the unwanted transition (i.e. it is not infinitely far off resonance). The post-selection procedure will remove any pairs from the ensemble which are affected by a microwave pulse, detuned or not; but of course this post-selection is ill-informed for those pairs in which the ancilla is incorrectly initialised. To allow for this one can simply expand the venality to include a fraction Δ of the inactive state population. Note that this Δ can be arbitrarily minimised in spin-resonance experiments by for example increasing the duration of the pulses which are applied, or using a sample with a larger splitting between the two microwave frequencies. In our experiment the Δ is less than 0.04 and we have confirmed that the corresponding correction to venality makes little difference to the degree of violation of our Leggett-Garg inequality.

Note that it is also important that the physical implementation of the CNOT (and anti-CNOT) operations is such that the primary system receives no perturbation when it is in state $\downarrow$; it would not be acceptable to implement the CNOT as a series of low level operations, some of which perturb the primary system: even if their net effect is that of the CNOT (as is the case for example with a controlled phase gate plus single qubit rotations).

SUPPLEMENTARY REFERENCES

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