No Fine Theorem for Macrorealism: Limitations of the Leggett-Garg Inequality

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Tests of local realism and macrorealism have historically been discussed in very similar terms: Leggett-Garg inequalities follow Bell inequalities as necessary conditions for classical behavior. Here, we compare the probability polytopes spanned by all measurable probability distributions for both scenarios and show that their structure differs strongly between spatially and temporally separated measurements. We arrive at the conclusion that, in contrast to tests of local realism where Bell inequalities form a necessary and sufficient set of conditions, no set of inequalities can ever be necessary and sufficient for a macrorealistic description. Fine's famous proof that Bell inequalities are necessary and sufficient for the existence of a local realistic model, therefore, cannot be transferred to macrorealism. A recently proposed condition, no-signaling in time, fulfills this criterion, and we show why it is better suited for future experimental tests and theoretical studies of macrorealism. Our work thereby identifies a major difference between the mathematical structures of local realism and macrorealism.

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The violation of classical world views, such as local realism [1] and macrorealism [2,3], is one of the most interesting properties of quantum mechanics. Experiments performed over the past decades have shown violations of local realism in various systems [4–6], while violations of macrorealism are on the horizon [7–24]. The latter endeavors pave the way towards the experimental realization of Schrödinger's famous thought experiment [25]. In the future, they might offer insight into important foundational questions, such as the quantum measurement problem [26], and allow experimental tests of (possibly gravitational) extensions of quantum mechanics [27].

Historically, the discussion of tests of macrorealism (MR) follows the discussion of tests of local realism (LR) closely: Leggett-Garg inequalities (LGIs) [2] are formulated similarly to Bell inequalities [1,28,29], and some concepts, e.g., quantum contextuality [30], are connected to both fields [31–35]. However, recently, a discrepancy between LR and MR has been identified: Whereas Fine's theorem states that Bell *inequalities* are both necessary and sufficient for LR [36], a combination of arrow of time (AoT) and no-signaling in time (NSIT) [37] *equalities* are necessary and sufficient for the existence of a macrorealistic description [38]. A previous study [38] also demonstrated that LGIs involving temporal correlation functions of pairs of measurements are not sufficient for macrorealism, but did not rule out a potential sufficiency of other sets of LGIs, e.g., of the Clauser-Horne (CH) type [29,39], leaving open the possibility of a Fine theorem for macrorealism. Moreover, cases have been identified where LGIs hide violations of macrorealism [31] that are detected by a simple NSIT condition [37]. The latter fails for totally mixed initial states, where a more involved NSIT condition is required [38]. These fundamental differences between tests of local realism and macrorealism seem connected to the peculiar definition of macrorealism [40,41].

In this Letter, we analyze the reasons for and the consequences of this difference. We show that the probability space spanned by quantum mechanics (QM) is of a higher dimension in a MR test than in a LR test, and we analyze the resulting structure of the probability polytope. We conclude that inequalities—excluding the pathological case of inequalities pairwise merging into equalities—are not suited to be sufficient conditions for MR, and they form only weak necessary conditions. Fine's theorem [36], therefore, cannot be transferred to macrorealism (unless one uses potentially negative quasiprobabilities [42]). Our study thus identifies a striking difference between the mathematical structures of LR and MR. While current experimental tests of macrorealism overwhelmingly use Leggett-Garg inequalities, this difference explains why NSIT is better suited to be a witness of nonclassicality; i.e., why it is violated for a much larger range of parameters [37,38].

Let us start by reviewing the structure of the LR polytope (LR), as described in Refs. [43–45]. Consider a LR test between $n \geq 2$ parties $i \in \{1, \ldots, n\}$. Each party can perform a measurement in one of the $m \geq 2$ settings $s_i \in \{1, \ldots, m\}$. Each setting has the same number $\Delta \geq 2$ of possible outcomes $q_i \in \{1, \ldots, \Delta\}$, and, to allow for all possible types of correlations, it may measure a distinct property of the system. We can define probability distributions $p_{q_1,\ldots,q_n|s_1,\ldots,s_n}$ for obtaining outcomes $q_1, \ldots, q_n$, given the measurement settings $s_1, \ldots, s_n$. If a party i chooses not to perform a measurement, the corresponding "setting" is labeled $s_i = 0$, and there is only one "outcome" labeled $q_i = 0$ (e.g., $p_{q_1,0|s_1,0}$ when only the first party performs a measurement). We leave out final zeros, e.g., $p_{q_1,\ldots,q_i,0,\ldots,0|s_1,\ldots,s_i,0,\ldots,0} = p_{q_1,\ldots,q_i|s_1,\ldots,s_i}$. Note that this convention differs from the literature for LR tests, where the case of no measurement is often left out [43,45], but simplifies the comparison between LR and MR tests. Each experiment is then completely described by $(m\Delta+1)^n$ probability distributions; it can be seen as a point in a probability space $\mathbb{R}^{(m\Delta+1)^n}$.

We now require normalization of the probabilities. There are $(m+1)^n$ linearly independent normalization conditions, as each probability only appears once:

$$\forall s_1,\ldots,s_n\colon \sum_{q_1,\ldots,q_n} p_{q_1,\ldots,q_n|s_1,\ldots,s_n} = 1. \tag{1}$$

Because of the special case of no measurements ($s_i = 0$), here (and in the following equations) we have abbreviated the notation of the summation: The possible values of q_i, in fact, depend on s_i. The normalization conditions reduce the dimension of the probability space to

$$(m\Delta+1)^n - (m+1)^n. \tag{2}$$

Furthermore, the positivity conditions

$$\forall s_1,\ldots,s_n,q_1,\ldots,q_n\colon p_{q_1,\ldots,q_n|s_1,\ldots,s_n} \geq 0 \tag{3}$$

restrict the reachable space to a subspace with the same dimension, but they are delimited by flat hyperplanes. The resulting subspace is called the *probability polytope* P.

In a LR test with spacelike separated parties, special relativity prohibits signaling from every party to any other,

$$\forall i,q_1,\ldots,q_{i-1},q_{i+1},\ldots,q_n,s_1,\ldots,s_n,s_i\neq 0\colon \tag{4}$$

$$p_{q_1,\ldots,q_{i-1},0,q_{i+1},\ldots,q_n|s_1,\ldots,s_{i-1},0,s_{i+1},\ldots,s_n} = \sum_{q_i=1}^{\Delta} p_{q_1,\ldots,q_n|s_1,\ldots,s_n}.$$

These *no-signaling* (NS) conditions restrict the probability polytope to a NS polytope (NS) of lower dimension. Taking their linear dependence, both amongst each other and with the normalization conditions, into account, we arrive at dimension [43]

$$\dim \mathsf{NS} = [m(\Delta-1)+1]^n - 1. \tag{5}$$

Since quantum mechanics obeys NS, and due to Tsirelson bounds [46], the space of probability distributions from spatially separated experiments implementable in quantum mechanics, $\mathsf{QM_S}$, is located strictly within the NS polytope. Furthermore, the space of local realistic probability distributions, LR, is a strict subspace of $\mathsf{QM_S}$. It is delimited by Bell inequalities (e.g., the CH and Clauser-Horne-Shimony-Holt inequalities for $n=m=\Delta=2$) and positivity conditions, and it therefore forms a polytope within $\mathsf{QM_S}$ [36,43]. In summary, we have $\mathsf{P}\supset\mathsf{NS}\supset\mathsf{QM_S}\supset\mathsf{LR}$, with $\dim\mathsf{P}>\dim\mathsf{NS}=\dim\mathsf{QM_S}=\dim\mathsf{LR}$. The structure of the NS, $\mathsf{QM_S}$, and LR spaces is sketched in the left panel of Fig. 1.

In a test of MR, temporal correlations take the role of a LR test's spatial correlations. Instead of spatially separated measurements on n systems by different observers, a single observer performs n sequential (macroscopically distinct) measurements on one and the same system. Again, each

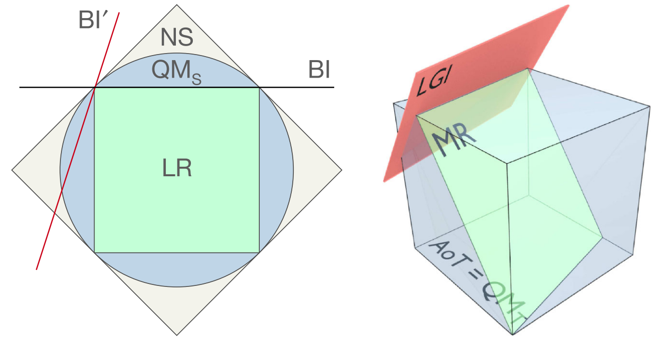

FIG. 1. (Left panel) A sketch of subspaces in a LR test [45]. The no-signaling polytope (NS) contains the space of probability distributions realizable from spatially separated experiments in quantum mechanics ($\mathsf{QM_S}$), which contains the local realism polytope (LR). LR is delimited by Bell inequalities and the positivity conditions. NS, QM_S, and LR have the same dimension. A Bell inequality (BI) is also sketched, delimiting LR. Another tight Bell inequality (BI′) is less suited to be a witness of non-LR behavior, and it illustrates the role of Leggett-Garg inequalities in macrorealism tests. (Right panel) A sketch of polytopes in a MR test. The arrow of time polytope (AoT) is equal to the space of probability distributions realizable from temporally separated experiments in quantum mechanics ($\mathsf{QM_T}$), which contains the macrorealism polytope (MR). MR is a polytope of lower dimension, located fully within the $\mathsf{QM_T}$ subspace and solely delimited by positivity constraints. Since each probability can easily be minimized or maximized individually, MR reaches all facets of AoT. A Leggett-Garg inequality (LGI) is also sketched; it is a hyperplane of dimension $\dim\mathsf{QM_T}-1$, which, in general, is much larger than $\dim\mathsf{MR}$. Note that the LGI can only touch MR (i.e., be tight) at the boundary of the positivity constraints.

measurement is either skipped ("0") or performed in one of the $m\geq 1$ [47] settings, with Δ possible outcomes each. With this one-to-one correspondence, the resulting probability polytope P in the space $\mathbb{R}^{(m\Delta+1)^n-(m+1)^n}$ is identical to the one in the Bell scenario. However, without further physical assumptions, no-signaling in temporally separated experiments is only a requirement in one direction: While past measurements can affect the future, causality demands that future measurements cannot affect the past. This assumption is captured by the AoT conditions:

$$\forall i\geq 2\colon\quad \forall\ q_1,\ldots,q_{i-1},s_1,\ldots,s_{i-1},\quad \text{with}$$
$$\Sigma_{j=1}^{i-1} s_j \neq 0, s_i\neq 0\colon$$

$$p_{q_1,\ldots,q_{i-1}|s_1,\ldots,s_{i-1}} = \sum_{q_i=1}^{\Delta} p_{q_1,\ldots,q_i|s_1,\ldots,s_i}. \tag{6}$$

Counting the number of equalities in Eq. (6) shows that their number is

$$\sum_{i=2}^{n}[(m\Delta+1)^{i-1}-1]m = \frac{(m\Delta+1)^n - nm\Delta - 1}{\Delta}, \tag{7}$$

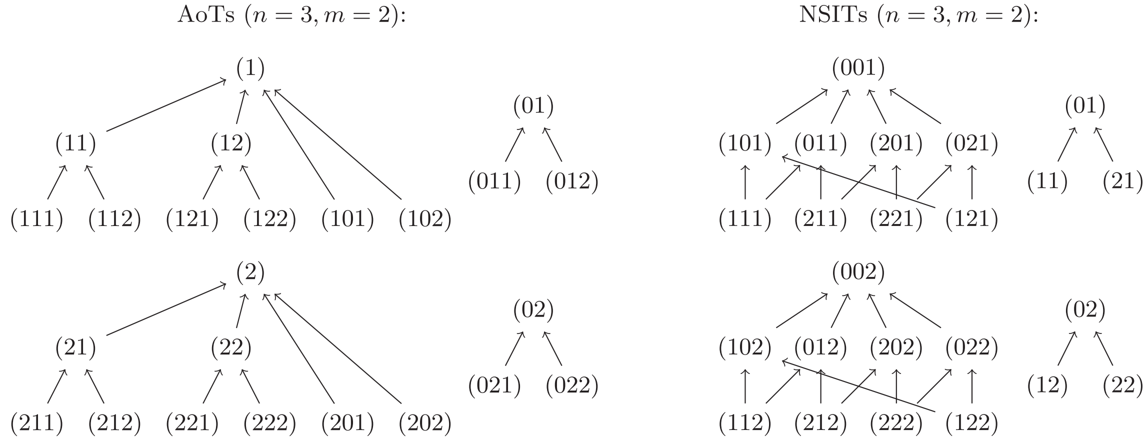

FIG. 2. Arrow of time (AoT) and no-signaling in time (NSIT) conditions relating different outcome probability distributions for the case $n = 3$ measurement times and $m = 2$ possible settings. The notation (xyz) refers to distributions with settings $s_1 = x, s_2 = y, s_3 = z$. The arrows denote the process of marginalization: For example, the AoT condition $p_{q_1|s_1=x} = \sum_{q_2} p_{q_1,q_2|s_1=x,s_2=y}$ is denoted by $(x) \leftarrow (xy)$, and the NSIT condition $p_{q_2|s_2=y} = \sum_{q_1} p_{q_1,q_2|s_1=x,s_2=y}$ is denoted by $(y) \leftarrow (xy)$. It can easily be seen that the AoT conditions are linearly independent since they cannot form loops. Adding more measurement times (adding further rows), or adding more settings (broadening the trees) does not change their independence. In contrast, the NSIT conditions are not linearly independent and thus form loops. Note that marginalizing only over a single measurement is sufficient, as simultaneous marginalizations follow from individual ones, and hence they are always linearly dependent.

where the first factor in the sum counts the setting and outcome combinations for times $1, \ldots, i-1$, excluding the choice of all $s_i = 0$, and the second factor the number of settings at time i. All listed conditions are linearly independent due to their hierarchical construction; see Fig. 2. However, a number of the normalization conditions for the marginal distributions, already subtracted in Eq. (2), are not linearly independent from AoT, and thus they become obsolete. Their number is obtained by counting the different settings in Eq. (6):

$$\sum_{i=2}^{n} [(m+1)^{i-1} - 1]m = (m+1)^n - nm - 1. \quad (8)$$

The remaining normalization conditions are the ones for probability distributions with just one measurement and for the "0 distribution"; there are $nm + 1$ such distributions. Taking Eq. (2), subtracting Eq. (7), and adding Eq. (8), we conclude that the AoT conditions restrict the probability polytope to an AoT polytope (AoT) of dimension

$$\dim \mathsf{AoT} = \frac{[(m\Delta + 1)^n - 1](\Delta - 1)}{\Delta}. \quad (9)$$

By simple extension of the proof in Ref. [38], the set of all NSIT conditions,

$$\forall i < n, q_1, \ldots, q_{i-1}, q_{i+1}, \ldots, q_n, s_1, \ldots, s_n, \Sigma_{j>i} s_j \neq 0, s_i \neq 0:$$

$$p_{q_1,\ldots,q_{i-1},0,q_{i+1},\ldots,q_n|s_1,\ldots,s_{i-1},0,s_{i+1},\ldots,s_n} = \sum_{q_i=1}^{\Delta} p_{q_1,\ldots,q_n|s_1,\ldots,s_n}, \quad (10)$$

is, together with AoT, necessary and sufficient for macrorealism. To get from AoT to the macrorealism polytope, MR, we therefore require a linearly independent subset of these conditions. However, since the AoT conditions from Eq. (6) plus the NSIT conditions from Eq. (10) are equivalent to the NS conditions from Eq. (4), we arrive at MR with the same dimension as the LR polytope:

$$\dim \mathsf{MR} = \dim \mathsf{LR} = [m(\Delta - 1) + 1]^n - 1. \quad (11)$$

We are left with the question of how the space of probability distributions realizable from temporally separated experiments in quantum mechanics, $\mathsf{QM_T}$, relates to AoT. Fritz has shown in Ref. [48] that $\mathsf{QM_T} = \mathsf{AoT}$ for $n = m = \Delta = 2$, if we allow for positive-operator valued measurements (POVMs). Let us now generalize his proof to arbitrary n, m, Δ's. We do so by constructing a quantum experiment that produces all possible probability distributions which are allowed by AoT.

Consider a quantum system of dimension $(m\Delta + 1)^n$, with states enumerated as $|q_1, \ldots, q_n; s_1, \ldots, s_n\rangle$. As with the probability distributions, final zeros may be omitted. The initial state of the system is $|0\ldots0; 0\ldots0\rangle$. Now, n POVMs are performed on the system. The measurements are chosen such that, depending on their setting and outcome, they take the system to the corresponding state: Performing a measurement on a system in state $|q_1, \ldots, q_{i-1}; s_1, \ldots, s_{i-1}\rangle$ with setting s_i and obtaining outcome q_i should leave the system in state $|q_1, \ldots, q_i; s_1, \ldots, s_i\rangle$. This is accomplished by choosing Kraus operators for the ith measurement in basis s_i for outcome q_i to be

$$K^{(i)}_{s_i,q_i} = \sum_{s_1,\ldots,s_{i-1},q_1,\ldots,q_{i-1}} \sqrt{r_{q_i|q_1,\ldots,q_{i-1},s_1,\ldots,s_i}} \times |q_1,\ldots,q_i;s_1,\ldots,s_i\rangle\langle q_1,\ldots,q_{i-1};s_1,\ldots,s_{i-1}| + \sum_{\substack{s_1,\ldots,s_n \\ q_1,\ldots,q_n \\ \Sigma_{j=i}^n s_j \neq 0}} \frac{1}{\sqrt{\Delta}} |q_1,\ldots,q_n;s_1,\ldots,s_n\rangle\langle q_1,\ldots,q_n;s_1,\ldots,s_n|. \tag{12}$$

For $i=1$, the first sum in Eq. (12) reduces to the single term $\sqrt{p_{q_1|s_1}}|q_1;s_1\rangle\langle 0\ldots 0;0\ldots 0|$, while the second sum remains unchanged. The second sum in Eq. (12) is necessary for the completeness relation $\sum_{q_i}(K^{(i)}_{s_i,q_i})^\dagger K^{(i)}_{s_i,q_i} = \mathbb{1}$. The above definitions also work for $s_i = 0$, where $r_{q_i=0|q_1,\ldots,q_{i-1},s_1,\ldots,s_{i-1},s_i=0} = 1$, and $(K^{(i)}_{s_i,q_i})^\dagger K^{(i)}_{s_i,q_i} = \mathbb{1}$. The conditional probabilities r in Eq. (12) can be obtained from the probabilities p using the assumption of AoT:

$$r_{q_i|q_1,\ldots,q_{i-1},s_1,\ldots,s_i} = \frac{p_{q_1,\ldots,q_i|s_1,\ldots,s_i}}{p_{q_1,\ldots,q_{i-1}|s_1,\ldots,s_{i-1}}}. \tag{13}$$

This construction gives a recipe to obtain any point in the AoT probability space in a quantum experiment. We have therefore shown that $\mathsf{AoT} = \mathsf{QM_T}$ for any choice of n, m, Δ.

Note that the probability distributions constructed above can also be achieved by a purely classical stochastic model, albeit with invasive measurements. Such an experiment would therefore not convince a macrorealist to give up his or her worldview. For that to happen, an experiment needs to properly address the clumsiness loophole [2,49,50]. The relevant methods previously established for the LGI can also be applied to NSIT-based experiments [24].

Since AoT is a polytope, $\mathsf{QM_T}$ with POVMs is also a polytope, and no nontrivial Tsirelson-like bounds exist. If, on the other hand, we only allowed projective measurements, we would have $\mathsf{QM_T} \subset \mathsf{AoT}$ with nontrivial Tsirelson-like bounds, as shown in Ref. [48]. In this case, $\mathsf{QM_T}$ would not be a polytope. It is easy to see that QM with projectors is unable to reproduce some probability distributions: $n=2, m=1, \Delta=2$, $p_{11|11}=1, p_{01|01}=0$ fulfills AoT but cannot be constructed in projective quantum mechanics since the initial state must be an eigenstate of the first measurement. Here, we consider the general case of POVMs.

In summary, we have

$$\begin{array}{ccccccc} \mathsf{P} & \supset & \mathsf{NS} & \supset & \mathsf{QM_S} & \supset & \mathsf{LR} \\ \| & & \cap & & \cap & & \cap \\ \mathsf{P} & \supset & \mathsf{AoT} & = & \mathsf{QM_T} & \supset & \mathsf{MR} \end{array}, \tag{14}$$

with $\mathsf{NS} = \mathsf{MR}$, and dimensions

$$\begin{array}{ccccccc} \dim\mathsf{P} & > & \dim\mathsf{NS} & = & \dim\mathsf{QM_S} & = & \dim\mathsf{LR} \\ \| & & \wedge & & \wedge & & \| \\ \dim\mathsf{P} & > & \dim\mathsf{AoT} & = & \dim\mathsf{QM_T} & > & \dim\mathsf{MR} \end{array}. \tag{15}$$

The structure of AoT, $\mathsf{QM_T}$ and MR within P is sketched on the right side of Fig. 1, the dimensions of all of the mentioned subspaces are printed in Table I.

Finally, let us compare the characteristics of quantum mechanics in LR and MR tests. Trivially, QM fulfills NS between spatially separated measurements, and AoT between temporally separated measurements [51]. While $\mathsf{QM_S}$ and LR have the same dimension and are separated by Bell inequalities, $\mathsf{QM_T}$ and MR span subspaces with different dimensions. Inequalities can never reduce the dimension of the probability space since they act as a hyperplane separating the fulfilling from the violating volume of probability distributions. We conclude that no combination of (Leggett-Garg) inequalities can be sufficient for macrorealism.

The observation that inequalities cannot be sufficient for macrorealism and the differences in the structure of the probability space shown above present fundamental discrepancies between LR and MR. Fine's observation [36] that Bell inequalities are necessary and sufficient for LR can therefore not be transferred to the case of LGIs and MR. More precisely, Fine's proof uses the implicit assumption of NS, which is obeyed by all reasonable physical theories, including QM. However, the temporal analogue to NS is the conjunction of AoT and NSIT, where AoT is obeyed by all reasonable physical theories, while NSIT is violated in QM. Therefore,

TABLE I. Dimensions of the probability space P and its subspaces reachable by spatially separated ($\mathsf{QM_S}$) or temporally separated ($\mathsf{QM_T}$) experiments in quantum mechanics, local realism (LR), and macrorealism (MR). There are n spatially or temporally separated measurements with m settings and Δ outcomes each.

	LR test		MR test
Number of unnormalized distributions		$(m\Delta+1)^n$	
$\dim\mathsf{P}$		$(m\Delta+1)^n-(m+1)^n$	
$\dim\mathsf{QM_S}$, $\dim\mathsf{QM_T}$	$[m(\Delta-1)+1]^n-1$	$<$	$[(m\Delta+1)^n-1](\Delta-1)/\Delta$
$\dim\mathsf{LR}$, $\dim\mathsf{MR}$		$[m(\Delta-1)+1]^n-1$	

$$\text{BIs} \underset{\not\Rightarrow}{\overset{\Leftarrow}{}} \text{LR} \Leftrightarrow \text{NS} \wedge \text{BIs} \tag{16}$$

$$\text{LGIs} \underset{\not\Rightarrow}{\overset{\Leftarrow}{}} \text{MR} \Leftrightarrow \text{AoT} \wedge \text{NSIT} \underset{\Rightarrow}{\overset{\not\Leftarrow}{}} \text{AoT} \wedge \text{LGIs}, \tag{17}$$

where "BIs" and "LGIs" denote the sets of all Bell and Leggett-Garg inequalities, respectively.

Moreover, since MR is a polytope with a smaller dimension than QM_T, LGIs can only touch MR (i.e., be *tight*) at one facet, i.e., a positivity constraint, as sketched in Fig. 1 on the right side. A comparable Bell inequality, sketched in Fig. 1 on the left as BI$'$, clearly illustrates the limitations resulting from this requirement. In an experimental test of MR, using a LGI, therefore, needlessly restricts the parameter space where violations can be found. The favorable experimental feasibility of NSIT is demonstrated by the theoretical analyses of Refs. [37,38], as well as the recent experiment of Ref. [24]. Note also the mathematical simplicity of the NSIT conditions when compared to the LGI. We conclude that, for further theoretical studies and future experiments, it might be advantageous to eschew the LGIs and rather use NSIT.

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two-particle state $\hat{\rho}_{12}$. We then calculate $\sum_{q_2} p_{q_1 q_2|s_1 s_2} = \sum_{q_2} \mathrm{tr}[(\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1} \otimes \hat{M}^{\dagger}_{q_2,s_2}\hat{M}_{q_2,s_2})\hat{\rho}_{12}] = \mathrm{tr}[(\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1} \otimes \mathbb{1}_2)\hat{\rho}_{12}] = \mathrm{tr}_1[\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1}\mathrm{tr}_2(\hat{\rho}_{12})] = \mathrm{tr}_1[\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1}\hat{\rho}_1] = p_{q_1|s_1}$. To show that QM fulfills AoT, we consider a setup where $\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1}$ are measured at time 1 on state $\hat{\rho}_1$, and $\hat{M}^{\dagger}_{q_2,s_2}\hat{M}_{q_2,s_2}$ are measured at time 2. We then have $\sum_{q_2} p_{q_1 q_2|s_1 s_2} = \sum_{q_2} \mathrm{tr}[\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1}\hat{\rho}_1]\mathrm{tr}[\hat{M}^{\dagger}_{q_2,s_2}\hat{M}_{q_2,s_2}\hat{\rho}_2^{q_1,s_1}] = \mathrm{tr}[\hat{M}^{\dagger}_{q_1,s_1}\hat{M}_{q_1,s_1}\hat{\rho}_1] = p_{q_1|s_1}$, where $\hat{\rho}_2^{q_1,s_1}$ is the state after measurement of s_1 at time 1 with outcome q_1, evolved to time 2. The proofs for more parties or more measurement times follow straightforwardly.