# Compatibility and noncontextuality for sequential measurements

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A basic assumption behind the inequalities used for testing noncontextual hidden variable models is that the observables measured on the same individual system are perfectly compatible. However, compatibility is not perfect in actual experiments using sequential measurements. We discuss the resulting "compatibility loophole" and present several methods to rule out certain hidden variable models that obey a kind of extended noncontextuality. Finally, we present a detailed analysis of experimental imperfections in a recent trapped-ion experiment and apply our analysis to that case.

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## I. INTRODUCTION

Since the early days of quantum mechanics (QM), it has been debated whether QM can be completed with additional hidden variables (HVs), which would eventually account for the apparent indeterminism of the results of single measurements in QM and may lead to a more detailed deterministic description of the world [1–3]. The problem of distinguishing QM from HV theories, however, cannot be addressed unless one makes additional assumptions about the structure of the HV theories. Otherwise, for a given experiment, one can just take the observed probability distributions as a HV model [4]. Moreover, there are explicit HV theories, such as Bohmian mechanics [5,6], which can reproduce all experiments up to date.

In the 1960s, it was learned that HV models reproducing the predictions of QM should have some peculiar and highly nonclassical properties. The most famous result in this direction is Bell's theorem [7]. Bell's theorem states that local HV models cannot reproduce the quantum-mechanical correlations between local measurements on some entangled states. In principle, the theorem just states a conflict between two descriptions of the world: QM and local HV models. However, the proof of Bell's theorem by means of an inequality involving correlations between measurements on distant systems, which is satisfied by any local HV model, but is violated by some quantum predictions [8], allows us to take a step further and test whether the world itself can be described by local HV models [9–13]. More recently, a similar approach has been used to test whether the world can be reproduced with some specific nonlocal HV models [14–16].

A second seminal result on HV models reproducing QM is the Kochen-Specker (KS) theorem [17–19]. To formulate it, one first needs the notion of compatible measurements: two or more measurements are compatible if they can be measured jointly on the same individual system without disturbing each other (i.e., without altering their results). Compatible measurements can be made simultaneously or in any order and can be repeated any number of times on the same individual system and always must give the same result independently of the initial state of the system.

Second, one needs the notion of noncontextuality. A context is a set of compatible measurements. A physical model is called noncontextual if it assigns to a measurement a result independent of which other compatible measurements are carried out. There are some scenarios where the assumption of noncontextuality is especially plausible, for instance, in the case of measurements on distant systems or in the case where the measurements concern different degrees of freedom of the same system and the degrees of freedom can be accessed independently.

In a nutshell, the KS theorem states that noncontextual HV models cannot reproduce QM. This impossibility occurs already for a single three-level system, so it is not related to entanglement.

There have been several proposals to test the KS theorem [20–24], but there also have been debates about whether the KS theorem can be experimentally tested at all [25–34]. Nevertheless, first experiments have been performed, but these experiments required some additional assumptions [35–38]. Furthermore, the notion of contextuality has been extended to state preparations [39] and experimentally investigated [40].

Quite recently, several inequalities have been proposed which hold for all noncontextual models, but are violated in QM, potentially allowing for a direct test [41–44]. A remarkable feature of some noncontextuality inequalities is that the violation is independent of the quantum state of the system [43,44]. In this article we will call these inequalities KS inequalities, since the proof of the KS theorem in Ref. [19] is also valid for any quantum state of the system. Very recently, several experiments have found violations of noncontextual inequalities [38,45–48]. Three of these experiments have found violations of a KS inequality for different states [45,46] or for a single (maximally mixed) state [48]. In these experiments, compatible observables are measured sequentially.

The measurements in any experiment are never perfect. In tests of noncontextuality inequalities, these imperfections

can be interpreted as a failure of the assumption that the observables measured sequentially on the same system are perfectly compatible. What if this compatibility is not perfect? We will refer to this problem as the "compatibility loophole." The main aim of this article is to give a detailed discussion of this loophole and demonstrate that, despite this loophole, classes of HV models which obey a generalized definition of noncontextuality can still be experimentally ruled out.

The article is organized as follows: In Sec. II we give precise definitions of compatibility and noncontextuality, focusing on the case of sequential measurements. We also review some inequalities which have been proposed to test noncontextual HV models.

In Sec. III we discuss the case of imperfectly compatible observables. We first derive an inequality which holds for any HV model; however, this inequality is not experimentally testable. Then, we consider several possible extensions of noncontextuality. By that, we mean replacing our initial assumption of noncontextuality for perfectly compatible observables with a new one, which covers also nearly compatible observables and implies the usual noncontextuality if the measurements are perfectly compatible. We then present several experimentally testable inequalities which hold for HV models with some generalized version of noncontextuality, but which are violated in QM. One of these inequalities has already been found to be violated in an experiment [45]. In Sec. IV we present details of this experiment.

In Sec. V we present two explicit contextual HV models which violate all investigated inequalities. These models, which do not satisfy the assumptions of extended noncontextuality, are useful in understanding which counterintuitive properties a HV model must have to reproduce the quantum predictions. Other contextual HV models for contextuality experiments have been proposed in Ref. [49]. Finally, in Sec. VI, we conclude and discuss consequences of our work for future experiments.

## II. HIDDEN VARIABLE MODELS AND NONCONTEXTUALITY

### A. Joint or sequential measurements

In the scenario originally used for discussing noncontextuality [19], a measurement device is treated as a single device producing outcomes for several compatible measurements (i.e., a context). When treating the measurement device in this manner, the whole context is needed to produce any output at all. In this joint measurement, one of the settings of the measurement device is always specifically associated with one of the outcomes, in the sense that another measurement device exists that takes only that setting as input and gives an identical outcome as output. This is checked by repeatedly making a joint measurement and the corresponding compatible single measurements in any possible order. This is at the basis of the noncontextuality argument. The argument goes as follows: *Precisely because* another contextless device exists that can measure the outcome of interest, there is good reason to assume that this outcome is independent of the context in the joint measurement.

In this article we discuss sequential individual measurements, rather than joint measurements. It might be argued that the version of the noncontextuality assumption needed in this scenario is more restrictive on the HV model than the version used for joint measurements. This would mean that a test using a sequential setup would be weaker than a test using a joint-measurement setup, because it would rule out fewer HV models. However, the motivation for assuming noncontextuality even in the joint-measurement setup is the existence of the individual measurements and their compatibility and repeatability when combined with joint context-requiring measurements. Therefore, the assumptions needed in the sequential-measurement setting are equally well motivated as the assumptions needed in the joint-measurement setting.

In fact, the sequential setting is closer to the actual motivation of assuming noncontextuality: There exist individual contextless measurement devices that give the same results as the joint measurements, and we actually use them in experiment. Furthermore, from an experimental point of view, a changed context in the joint-measurement device corresponds to a physically entirely different setup even for the unchanged setting within the context, so it is difficult to maintain that the outcome for the unchanged setting is unchanged from physical principles [18,50]. Motivating physically unchanged outcomes is much easier in the sequential setup, since the device used is physically identical for the unchanged setting.

Therefore, in this article we consider the situation where sequences of measurements are made on an individual physical system. Throughout the article, we consider only dichotomic measurements with outcomes $\pm 1$, but the results can be generalized to arbitrary measurements. The question is: Under which conditions can the results of such measurements be explained by a HV model? More precisely, we ask which conditions a HV model has to violate in order to reproduce the quantum predictions.

### B. Notation

The following notation will be used in the discussed HV models: $\lambda$ is the HV, drawn with a distribution $p(\lambda)$ from a set $\Lambda$. The distribution summarizes all information about the past, including all preparation steps and all measurements already performed. Causality is assumed, so the distribution is independent of any event in the future. It rather determines all the probabilities of the results of all possible future sequences of measurements. We assume that, for a fixed value of the HV, the outcomes of future sequences of measurements are deterministic; hence, all indeterministic behavior stems from the probability distribution. This is similar to the investigation of Bell inequalities, where any stochastic HV model can be mapped onto a deterministic one where the HV is not known [4,51].

In an experiment, one first prepares a "state" via certain preparation procedures (which may include measurements). One always regards a state preparation as a procedure that can be repeated. At the HV level, it will therefore lead to an experimentally accessible probability distribution $p_{\text{expt}}(\lambda)$. The HV model hence enables the experimenter to repeatedly prepare the same distribution. In a single instance of an

experiment, one obtains a state determined by a single value $\lambda$ of the HV. The probability for this instance is distributed according to the distribution $p_{\text{expt}}(\lambda)$ and reflects the inability of the experimenter to control which particular value of the HVs has been prepared in a single instance.

Continuing, we denote by $A_i$ the measurement of the observable (or measurement device) $A$ at the position $i$ in the sequence. For example, $A_1 B_2 C_3$ denotes the sequence of measuring $A$ first, then $B$, and finally $C$. An outcome from a measurement of, for example, $B_2$ from the preceding sequence is denoted $v(B_2|A_1B_2C_3)$. The product of three outcomes is denoted $v(A_1B_2C_3) = v(A_1|A_1B_2C_3)v(B_2|A_1B_2C_3)v(C_3|A_1B_2C_3)$. Given a probability distribution $p(\lambda)$, we write probabilities $p(B_2^+|A_1B_2C_3)$ [or $p(B_2^+C_3^-|A_1B_2C_3)$] for the probability of obtaining the value $B_2 = +1$ (and $C_3 = -1$) when the sequence $A_1B_2C_3$ is measured. One can also consider mean values like $\langle B_2|A_1B_2C_3\rangle = p(B_2^+|A_1B_2C_3) - p(B_2^-|A_1B_2C_3)$ or the mean value of the complete sequence, $\langle A_1B_2C_3\rangle = p[v(A_1B_2C_3) = +1] - p[v(A_1B_2C_3) = -1]$.

### C. Compatibility of measurements

In the simplest case, compatibility is a relation between a pair of measurements, $A$ and $B$. For that, let $\mathcal{S}_{AB}$ denote the (infinite) set of all sequences that use only measurements of $A$ and $B$; that is, $\mathcal{S}_{AB} = \{A_1, B_1, A_1A_2, A_1B_2, B_1A_2, \ldots\}$. Then we formulate the following.

*Definition 1.* Two observables $A$ and $B$ are compatible if the following two conditions are fulfilled:

(i) For any instance of a state (i.e., for any $\lambda$) and for any sequence $S \in \mathcal{S}_{AB}$, the obtained values of $A$ and $B$ remain the same,

$$v(A_k|S) = v(A_l|S), \tag{1a}$$

$$v(B_m|S) = v(B_n|S), \tag{1b}$$

where $k$, $l$, $m$, and $n$ are all possible indices for which the considered observable is measured at the positions $k$, $l$, $m$, and $n$ in the sequence $S$. [Equivalently, we could require that $p(A_k^+A_l^-|S) = 0$, etc., for all preparations corresponding to some $p_{\text{expt}}(\lambda)$.]

(ii) For any state preparation [i.e., for any $p_{\text{expt}}(\lambda)$], the mean values of $A$ and $B$ during the measurement of any two sequences $S_1$, $S_2 \in \mathcal{S}_{AB}$ are equal,

$$\langle A_k|S_1\rangle = \langle A_l|S_2\rangle, \tag{2a}$$

$$\langle B_m|S_1\rangle = \langle B_n|S_2\rangle. \tag{2b}$$

Clearly, conditions (i) and (ii) are necessary conditions for compatible observables in the sense that two observables which violate any of them cannot reasonably called compatible.

It is important to note that the compatibility of two observables is experimentally testable by repeatedly preparing all possible $p_{\text{expt}}(\lambda)$. The fact that this set is infinite is not a specific problem here, as any measurement device or physical law can only be tested in a finite number of cases. A crucial point in a HV model is that the set of all experimentally accessible probability distributions $p_{\text{expt}}(\lambda)$ might not coincide with the set of all possible distributions $p(\lambda)$. We will discuss this issue in Sec. III D.

It should be noted that the conditions (i) and (ii) are not minimal (cf. the Appendix for a discussion). In particular, we emphasize that (ii) does not necessarily follow from (i), as we illustrate by the following example: Consider a HV model where, for any $\lambda$, all $v(A_k|S)$ are $+1$ when the first measurement in $S$ is $A_1$, while they are $-1$ when the first measurement is $B_1$. The values $v(B_m|S)$ are always $+1$. Then condition (i) is fulfilled while (ii) is violated, since $\langle A\rangle = 1$ but $\langle A_2|B_1A_2\rangle = -1$.

Let us compare our definition of compatibility to the notion of "equivalent measurements" introduced by Spekkens in Ref. [39]. In this reference, two measurements are called equivalent if, for any state preparation, the probability distributions of the measurement outcomes for both measurements are the same. This is similar to our condition (ii) but disregards repeated measurements on individual systems as in (i). Interestingly, using this notion and positive operator-valued measures (POVMs), one can prove the contextuality of a quantum-mechanical two-level system [39].

Finally, it should be added that the notion of compatibility is extended in a straightforward manner to three or more observables. For instance, if three observables $A$, $B$, and $C$ are investigated, one considers the set $\mathcal{S}_{ABC}$ of all measurement sequences involving measurements of $A$, $B$, or $C$ and extends the conditions (i) and (ii) in an obvious way. This is equivalent to requiring the pairwise compatibility of $A$, $B$, and $C$ (cf. the Appendix).

### D. Definition of noncontextuality for sequential measurements

Noncontextuality means that the value of any observable $A$ does not depend on which other compatible observables are measured jointly with $A$. For our models, we formulate noncontextuality as a condition on a HV model as follows.

*Definition 2.* Let $A$ and $B$ be observables in a HV model, where $A$ is compatible with $B$. We say that the HV model is noncontextual if it assigns, for any $\lambda$, an outcome of $A$ which is independent of whether $B$ is measured before or after $A$, that is,

$$v(A_1) = v(A_2|B_1A_2). \tag{3}$$

Hence, for these sequences we can write $v(A)$ as being independent of the sequence. If the condition is not fulfilled, we call the model contextual.

It is important to note that the condition (3) is an assumption about the model and—contrary to the definition of compatibility—not experimentally testable. This is due to the fact that for a given instance of a state (corresponding to some unknown $\lambda$) the experimenter has to decide whether to measure $A$ or $B$ first.

From this definition and the time ordering, it follows immediately that, if $A$ is compatible with $B$ and $A$ is also compatible with $C$, then for noncontextual models

$$v(A_1|A_1B_2) = v(A_2|B_1A_2) = v(A_1|A_1C_2) = v(A_2|C_1A_2)$$

$$\tag{4}$$

holds. This is the often-used definition of noncontextual models, stating that the value of $A$ does not depend on whether $B$ or $C$ is measured before, jointly with, or after it.

This definition can directly be extended to three or more compatible observables. For instance, if $\{A, B, C\}$ are compatible, then noncontextuality means that for any $\lambda$,

$$
\begin{aligned}
v(A_1) &= v(A_2|B_1A_2) = v(A_2|C_1A_2) \\
&= v(A_3|B_1B_2A_3) = v(A_3|B_1C_2A_3) \\
&= v(A_3|C_1B_2A_3) = v(A_3|C_1C_2A_3).
\end{aligned} \tag{5}
$$

Of course, the equalities in the second and third lines follow if the first line holds for any $\lambda$ and the HV model allows the measurement of $B_1$ or $C_1$ to be seen as a preparation step. Again, if $\{A, a, \alpha\}$ is another set of compatible observables, one can derive consequences similar to Eq. (4).

### E. Inequalities for noncontextual HV models

Here we will discuss several previously introduced inequalities involving compatible measurements, which hold for any noncontextual HV model, but which are violated for certain states and observables in QM. Later, these inequalities are extended to the case where the observables are not perfectly compatible.

#### 1. Clauser-Horne-Shimony-Holt (CHSH)-like inequality

To derive a first inequality, consider the mean value

$$
\langle \chi_{\mathrm{CHSH}} \rangle = \langle AB \rangle + \langle BC \rangle + \langle CD \rangle - \langle DA \rangle. \tag{6}
$$

If the measurements in each average are compatible [i.e., the pairs $(A, B)$, $(B, C)$, $(C, D)$, and $(D, A)$ are compatible observables)], then a noncontextual HV model has to assign a fixed value to each measurement, and the model predicts

$$
|\langle \chi_{\mathrm{CHSH}} \rangle| \leqslant 2. \tag{7}
$$

In QM, on a two-qubit system, one can take the observables

$$
\begin{aligned}
A &= \sigma_x \otimes \mathbb{1}, & B &= \mathbb{1} \otimes \frac{(\sigma_z + \sigma_x)}{\sqrt{2}}, \\
C &= \sigma_z \otimes \mathbb{1}, & D &= \mathbb{1} \otimes \frac{(\sigma_z - \sigma_x)}{\sqrt{2}},
\end{aligned} \tag{8}
$$

then the measurements in each sequence are commuting and hence compatible, but the state

$$
|\phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2} \tag{9}
$$

leads to a value of $\langle \chi_{\mathrm{CHSH}} \rangle = 2\sqrt{2}$, therefore not allowing any noncontextual description. The choice of the observables in Eq. (8) is, however, by no means unique, if one transforms all of them via the same global unitary transformation, another set is obtained, and the state leading to the maximal violation does not need to be entangled. In fact, the two-qubit notation is only chosen for convenience and could be replaced with a formulation with a single party using a four-level system. For example, if we take the observables

$$
A = \sigma_x \otimes \sigma_x, \qquad B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix},
$$

$$
C = \sigma_z \otimes \mathbb{1}, \qquad D = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}, \tag{10}
$$

then the measurements in each sequence are commuting and hence compatible, but the product state

$$
|\Psi\rangle = |x^+\rangle|0\rangle = (|00\rangle + |10\rangle)/\sqrt{2} \tag{11}
$$

leads to a value of $\langle \chi_{\mathrm{CHSH}} \rangle = 2\sqrt{2}$, therefore not allowing any noncontextual description.

#### 2. The Klyachko, Can, Binicioğlu, and Shumovsky (KCBS) inequality

As a second inequality, we take the pentagram inequality introduced by Klyachko, Can, Binicioğlu, and Shumovsky [42]. Here, one takes five dichotomic observables and considers

$$
\langle \chi_{\mathrm{KCBS}} \rangle = \langle AB \rangle + \langle BC \rangle + \langle CD \rangle + \langle DE \rangle + \langle EA \rangle. \tag{12}
$$

If the observables in each mean value are compatible and noncontextuality is assumed, it can be seen that

$$
\langle \chi_{\mathrm{KCBS}} \rangle \geqslant -3 \tag{13}
$$

holds. However, using appropriate measurements on a three-level system, there are qutrit states which give a value of $\langle \chi_{\mathrm{KCBS}} \rangle = 5 - 4\sqrt{5} \approx -3.94$, also leading to contradiction with noncontextuality.

#### 3. An inequality from the Mermin-Peres square

For the third inequality, we take the one introduced in Ref. [43]. Consider the mean value

$$
\begin{aligned}
\langle \chi_{\mathrm{KS}} \rangle = {} & \langle ABC \rangle + \langle abc \rangle + \langle \alpha\beta\gamma \rangle + \langle Aa\alpha \rangle \\
& + \langle Bb\beta \rangle - \langle Cc\gamma \rangle.
\end{aligned} \tag{14}
$$

If the measurements in each expectation value are compatible, then any noncontextual HV model has to assign fixed values to each of the nine occurring measurements. Then, one can see that

$$
\langle \chi_{\mathrm{KS}} \rangle \leqslant 4. \tag{15}
$$

However, on a two-qubit system, one can choose the observables of the Mermin-Peres square [52,53]

$$
\begin{aligned}
A &= \sigma_z \otimes \mathbb{1}, & B &= \mathbb{1} \otimes \sigma_z, & C &= \sigma_z \otimes \sigma_z, \\
a &= \mathbb{1} \otimes \sigma_x, & b &= \sigma_x \otimes \mathbb{1}, & c &= \sigma_x \otimes \sigma_x, \\
\alpha &= \sigma_z \otimes \sigma_x, & \beta &= \sigma_x \otimes \sigma_z, & \gamma &= \sigma_y \otimes \sigma_y.
\end{aligned} \tag{16}
$$

The observables in any row or column commute and are therefore compatible. Moreover, the product of the observables in any row or column equals $\mathbb{1}$, apart from the rightmost column, where it equals $-\mathbb{1}$. Hence, for any quantum state,

$$
\langle \chi_{\mathrm{KS}} \rangle = 6 \tag{17}
$$

holds. The remarkable fact in this result is that it shows that any quantum state reveals nonclassical properties if the measurements are chosen appropriately.

## III. NOT PERFECTLY COMPATIBLE MEASUREMENTS

In any real experiment, the measurements will not be perfectly compatible. Hence, the notion of noncontextuality does not directly apply. The experimental violation of inequalities like (7), (13), and (15) proves that one cannot assign to the measurement devices independent outcomes $\pm 1$. However, a model that is not trivially in conflict with QM also has to explain the measurement results of sequences of incompatible observables, such as, for example, the results from measuring $A_1 C_2$ for the observables of the CHSH-like inequality. Therefore, it is not straightforward to find out what the implications of these violations on the structure of the possible HV models are. The reason is that the assumption that incompatible measurements have predetermined independent outcomes is not physically plausible.

To deal with this problem, we will derive extended versions of the inequalities (7), (13), and (15), which are valid even in the case of imperfect compatibility. We will first derive an inequality which is an extension of inequality (7) and which holds for any HV model. This inequality, however, contains terms which are not experimentally accessible. Then, we investigate how these terms can be connected to experimental quantities, if certain assumptions about the HV model are made. We will present three types of testable inequalities, the first two start from condition (i) of Definition 1, while the third one uses condition (ii).

First we consider nearly compatible observables. We show that if the observables fulfill the condition (i) of Definition 1 to some extent and if assumptions about the dynamics of probabilities in a HV model are made, then these HV models can be experimentally refuted.

In the second approach, we consider the case that a certain finite number of compatibility tests has been made. For some runs of the experiment the tests are successful [i.e., no error occurs when checking condition (i)], and in some runs errors occur. We then assume that the subset of HVs where noncontextuality holds is at least as large as the subset where the compatibility tests are successful. We then show that HV models of this type can, in principle, be refuted experimentally.

Finally, in the third approach, we also consider assumptions about the possible distributions $p_{\text{expt}}(\lambda)$ and show that if the condition (ii) of Definition 1 is nearly fulfilled, then again this type of HV model can experimentally be ruled out.

We will discuss these approaches using the CHSH-like inequality (7). At the end of the section, we will also explain how the inequalities (13) and (15) have to be modified, in order to test these different types of HV models.

### A. CHSH-like inequality for all HV models

To start, consider a HV model with a probability distribution $p(\lambda)$ and let $p[(A_1^+|A_1)$ and $(B_1^+|B_1)]$ denote the probability of finding $A^+$ if $A$ is measured first and $B^+$ if $B$ is measured first. This probability is well defined in all HV models of the considered type, but it is impossible to measure it directly, as one has to decide whether one measures $A$ or $B$ first. Our aim is now to connect it to probabilities arising in sequential measurements, as this will allow us to find contradictions between HV models and QM.

First, note that

$$p[(A_1^+|\ A_1) \text{ and } (B_1^+|B_1)] \leqslant p[A_1^+, B_2^+|A_1 B_2]$$
$$+ p[(B_1^+|B_1) \text{ and } (B_2^-|A_1 B_2)]. \quad (18)$$

This inequality is valid because if $\lambda$ is such that it contributes to $p[(A_1^+|A_1)$ and $(B_1^+|B_1)]$, then either the value of $B$ stays the same when measuring $A_1 B_2$ (hence $\lambda$ contributes to $p[A_1^+, B_2^+|A_1 B_2]$) or the value of $B$ is flipped and $\lambda$ contributes to $p[(B_1^+|B_1)$ and $(B_2^-|A_1 B_2)]$. The first term $p[A_1^+, B_2^+|A_1 B_2]$ is directly measurable as a sequence, but the second term is not experimentally accessible.

Let us rewrite

$$\langle AB \rangle = 1 - 2p[(A_1^+|A_1) \text{ and } (B_1^-|B_1)]$$
$$- 2p[(A_1^-|A_1) \text{ and } (B_1^+|B_1)] \quad (19)$$

as the mean value obtained from the probabilities $p[(A_1^\pm|A_1)$ and $(B_1^\pm|B_1)]$. Then, using Eq. (18), it follows that

$$\langle A_1 B_2 \rangle - 2p^{\text{flip}}[AB] \leqslant \langle AB \rangle \leqslant \langle A_1 B_2 \rangle + 2p^{\text{flip}}[AB], \quad (20)$$

where we used $p^{\text{flip}}[AB] = p[(B_1^+|B_1)$ and $(B_2^-|A_1 B_2)] + p[(B_1^-|B_1)$ and $(B_2^+|A_1 B_2)]$. This $p^{\text{flip}}[AB]$ can be interpreted as a probability that $A$ flips a predetermined value of $B$.

Furthermore, using Eqs. (6) and (7), we obtain

$$|\langle \mathcal{X}_{\text{CHSH}} \rangle| \leqslant 2(1 + p^{\text{flip}}[AB] + p^{\text{flip}}[CB]$$
$$+ p^{\text{flip}}[CD] + p^{\text{flip}}[AD]), \quad (21)$$

where

$$\langle \mathcal{X}_{\text{CHSH}} \rangle := \langle A_1 B_2 \rangle + \langle C_1 B_2 \rangle + \langle C_1 D_2 \rangle - \langle A_1 D_2 \rangle. \quad (22)$$

Inequality (21) holds for any HV model and is the generalization of inequality (7). Note that for perfectly compatible observables, the flip terms in inequality (21) vanish if the assumption of noncontextuality is made. Then this results in inequality (7).

### B. First approach: Constraints on the disturbance and the dynamics of the HV

The terms $p^{\text{flip}}[AB]$, etc., in inequality (21) are not experimentally accessible. Now we will discuss how they can be experimentally estimated when some assumptions on the HV model are made.

In order to obtain an experimentally testable version of inequality (21), we will assume that

$$p[(B_1^+ B_1) \text{ and } (B_2^-|A_1 B_2)]$$
$$\leqslant p[(B_1^+|B_1) \text{ and } (B_1^+, B_3^-|B_1 A_2 B_3)]$$
$$\equiv p[B_1^+, B_3^-|B_1 A_2 B_3]. \quad (23)$$

This assumption is motivated by the experimental procedure: Let us assume that one has a physical state, for which one surely finds $B_1^+$ if $B_1$ is measured first, but finds $B_2^-$ if the sequence $A_1 B_2$ is measured. Physically, one would explain this behavior as a disturbance of the system due to the experimental procedures when measuring $A_1$. The left-hand side of Eq. (23) can be viewed as the amount of this disturbance. The right-hand side quantifies the disturbance of $B$ when the sequence $B_1 A_2 B_3$ is measured. In real experiments, it can be expected that this disturbance is larger than when measuring $A_1 B_2$, because of the additional experimental procedures involved.

Note that in real experiments, a measurement of $B$ will also disturb the value of $B$ itself, as can be seen from the fact that sometimes the values of $B_1$ and $B_2$ will not coincide, if the sequence $B_1B_2$ is measured.

It should be stressed, however, that we do not assume that the set of HV values giving $[(B_1^+|B_1)$ and $(B_2^-|A_1B_2)]$ is contained in the set giving $(B_1^+, B_3^-|B_1A_2B_3)$; the assumption only relates the sizes of these two sets.

In addition, by similar reasoning, assumption (23) may be relaxed to

$$p[(B_1^+|B_1) \text{ and } (B_2^-|A_1B_2)] \leqslant p[B_1^+, B_k^-|B_1SA_{k-1}B_k], \tag{24}$$

where $S$ is a given finite sequence of measurements from $\mathcal{S}_{AB}$. Again, if the measurements are nearly compatible, this type of HV model can be ruled out experimentally.

Assumption (23) gives an measurable upper bound to $p^{\text{flip}}[AB]$. One directly has

$$|\langle \mathcal{X}_{\text{CHSH}} \rangle| \leqslant 2(1 + p^{\text{err}}[B_1A_2B_3] + p^{\text{err}}[B_1C_2B_3]$$
$$+ p^{\text{err}}[D_1C_2D_3] + p^{\text{err}}[D_1A_2D_3]), \tag{25}$$

where we used

$$p^{\text{err}}[B_1A_2B_3] = p[B_1^+, B_3^-|B_1A_2B_3]$$
$$+ p[B_1^-, B_3^+|B_1A_2B_3], \tag{26}$$

denoting the total disturbance probability of $B$ when measuring $B_1A_2B_3$.

The point of this inequality is that if the observable pairs $(A, B)$, $(C, B)$, $(C, D)$, and $(A, D)$ fulfill approximately the condition (i) in the definition of compatibility, the terms $p^{\text{err}}$ will become small, and a violation of inequality (25) can be observed. In Ref. [45] it was found that $\langle \mathcal{X}_{\text{CHSH}} \rangle - 2(p^{\text{err}}[B_1A_2B_3] + p^{\text{err}}[B_1C_2B_3] + p^{\text{err}}[D_1C_2D_3] + p^{\text{err}}[D_1A_2D_3]) = 2.23(5)$. Hence, this experiment cannot be described by HV models which fulfill Eq. (23) (see also Sec. IV).

### C. Second approach: Assuming noncontextuality for the set of HVs where the observables are compatible

Let us discuss a different approach to obtaining experimentally testable inequalities. For that, consider the case that the experimenter has measured a (finite) set of sequences in $\mathcal{S}_{AB}$ in order to test the validity of condition (i) in the definition of compatibility. He finds that the conditions are violated or fulfilled with certain probabilities. In terms of the HV model, there is a certain subset $\Lambda_{AB} \subset \Lambda$ of all HVs where *all* tests in the finite set of experimentally performed compatibility tests succeed and where through the observed probabilities the experimenter can estimate the volume of this set.

In this situation, one can assume that, for each HV $\lambda \in \Lambda_{AB}$ (where all the measured compatibility requirements are fulfilled), the assumption of noncontextuality is also valid. More precisely, one can assume that $v(A_1|A_1B_2) = v(A_2|B_1A_2)$ in Eq. (3) holds for all $\lambda \in \Lambda_{AB}$. One may support this assumption if one considers noncontextuality as a general property of nature, since this is the usual noncontextuality assumption for the HV model where the HVs are restricted to $\Lambda_{AB}$.

To see that this assumption leads to an experimentally testable inequality, consider the case where the experimenter has tested all sequences up to length 3, that is all sequences from $\mathcal{S}_{AB}^{(3)} = \{A_1A_2A_3, A_1A_2B_3, \ldots, B_1B_2B_3\}$, and has determined, for each of them, the probability $p^{\text{err}}(S)$ that some measurement, which is performed two or three times in the sequence, is disturbed. For sequences like $B_1A_2B_3$, this is exactly $p^{\text{err}}[B_1A_2B_3]$ defined in Eq. (26). However, now we have additional error terms like $p^{\text{err}}[B_1B_2A_3] = p[B_1^+, B_2^-|B_1B_2A_3] + p[B_1^-, B_2^+|B_1B_2A_3]$, $p^{\text{err}}[B_1B_2B_3] = 1 - p[B_1^+, B_2^+B_3^+|B_1B_2B_3] - p[B_1^-, B_2^-B_3^-|B_1B_2B_3]$, etc. These probabilities are not completely independent: Due to the time ordering, a $\lambda$ that contributes to $p^{\text{err}}[B_1B_2A_3]$ (or $p^{\text{err}}[A_1A_2B_3]$) will also contribute to $p^{\text{err}}[B_1B_2B_3]$ (or $p^{\text{err}}[A_1A_2A_3]$). Consequently, relations like $p^{\text{err}}[B_1B_2A_3] \leqslant p^{\text{err}}[B_1B_2B_3]$ hold.

Let us define

$$p^{\text{err}}[\mathcal{S}_{AB}^{(3)}] = \left( \sum_{S \in \mathcal{S}_{AB}^{(3)}} p^{\text{err}}[S] \right) - p^{\text{err}}[B_1B_2A_3]$$
$$- p^{\text{err}}[A_1A_2B_3]. \tag{27}$$

Here, we have excluded two $p^{\text{err}}$ in the sum, as the $\lambda$'s which contribute to them are already counted in other terms. With this definition, for a given distribution $p_{\text{expt}}(\lambda)$, a lower bound to the probability of finding a $\lambda$ where condition (i) from Definition 1 is fulfilled is

$$p[\Lambda_{AB}] \geqslant 1 - p^{\text{err}}[\mathcal{S}_{AB}^{(3)}]. \tag{28}$$

From that and the assumption that $v(A_1|A_1B_2) = v(A_2|B_1A_2)$ on $\Lambda_{AB}$, it directly follows that

$$p^{\text{flip}}[AB] \leqslant p^{\text{err}}[\mathcal{S}_{AB}^{(3)}], \tag{29}$$

giving a measurable upper bound to $p^{\text{flip}}[AB]$. Finally, the experimentally testable inequality

$$|\langle \mathcal{X}_{\text{CHSH}} \rangle| \leqslant 2(1 + p^{\text{err}}[\mathcal{S}_{AB}^{(3)}] + p^{\text{err}}[\mathcal{S}_{CB}^{(3)}]$$
$$+ p^{\text{err}}[\mathcal{S}_{CD}^{(3)}] + p^{\text{err}}[\mathcal{S}_{AD}^{(3)}]) \tag{30}$$

holds. This inequality is similar to inequality (25), but it contains more error terms. Nevertheless, a violation of this inequality in ion-trap experiments might be feasible in the near future (see Sec. IV).

This result deserves two further comments. First, in the derivation we assumed a pointwise relation; namely, for all $\lambda \in \Lambda_{AB}$, the noncontextuality assumption $v(A_1|A_1B_2) = v(A_2|B_1A_2)$ holds. Of course, we could relax this assumption by assuming only that the volume of the set where $v(A_1|A_1B_2) = v(A_2|B_1A_2)$ holds is not smaller than the volume of $\Lambda_{AB}$. Under this condition, Eq. (30) still holds.

Second, when comparing the second approach with the first one, one finds that the first one is indeed a special case of the second one. In fact, from a mathematical point of view, the first approach is the same as the second one, if in the second approach only the compatibility test $S = B_1A_2B_3$ is performed. Consequently, inequality (25) is weaker than (30). However, note that the first approach came from a different physical motivation. Further, assuming a pointwise relation for the first approach is very assailable, as only one compatibility

test is made. However, as we have seen, a relation between the volumes suffices. A pointwise relation can only be motivated if all experimentally feasible compatibility tests are performed.

### D. Third approach: Certain probability distributions cannot be prepared

The physical motivation of the third approach is as follows: The experimenter can prepare different probability distributions $p_{\text{expt}}(\lambda)$ and check their properties. For instance, he or she can test to what extent the condition (ii) in Definition 1 is fulfilled. However, in a general HV model there might be probability distributions $p(\lambda)$ that do not belong to the set of experimentally accessible $p_{\text{expt}}(\lambda)$. One might be tempted to believe that this difference is negligible and that the properties that can be verified for the $p_{\text{expt}}(\lambda)$ hold also for some of the $p(\lambda)$. In this approach we will show that this belief can be experimentally falsified. More specifically, we show that if only four conditional probability distributions have the same properties as all $p_{\text{expt}}(\lambda)$, then a contradiction with QM occurs.

So let us assume that the experimenter has checked that the observables $A$ and $B$ fulfill condition (ii) in Definition 1 approximately. He has found that

$$|\langle B_1|B_1 A_2\rangle - \langle B_2|A_1 B_2\rangle| \leqslant \varepsilon_{AB} \qquad (31)$$

for all possible (or at least a large number of) $p_{\text{expt}}(\lambda)$. This means that, for experimentally accessible distributions $p_{\text{expt}}(\lambda)$, one has that

$$|p(B_1^+|B_1 A_2) - p(B_2^+|A_1 B_2)| \leqslant \varepsilon_{AB}/2,$$
$$|p(B_1^-|B_1 A_2) - p(B_2^-|A_1 B_2)| \leqslant \varepsilon_{AB}/2, \qquad (32)$$

as can be seen by direct calculation.

Let us consider the flip probability $p^{\text{flip}}[AB] = p[(B_1^+|B_1) \text{ and } (B_2^-|A_1 B_2)] + p[(B_1^-|B_1) \text{ and } (B_2^+|A_1 B_2)]$ again. Here, the probability $p$ stems from the initial probability distribution $p(\lambda)$. One can consider the conditional probability distributions $q^{\pm}(\lambda)$ which arise from $p(\lambda)$ if the result of $B_1$ is known. Physically, the conditional distributions describe the situation for an observer who knows that the experimenter has prepared $p(\lambda)$ but has the additional information that measurement of $B_1$ will give $+1$ or $-1$. With that, we can rewrite

$$p^{\text{flip}}[AB] = q^+(B_2^-|A_1 B_2)p(B_1^+|B_1)$$
$$+ q^-(B_2^+|A_1 B_2)p(B_1^-|B_1). \qquad (33)$$

Now let us assume that these conditional probability distributions have the same properties as all accessible distributions $p_{\text{expt}}(\lambda)$. Then, the bounds in Eq. (32) also have to hold for $q^{\pm}$. Since $p(B_1^+|B_1) + p(B_1^-|B_1) = 1$, it follows directly that $p^{\text{flip}}[AB] \leqslant \varepsilon_{AB}/2$. Hence, under the assumption that some conditional probability distributions in the HV model have properties similar to those of the preparable $p_{\text{expt}}(\lambda)$, the inequality

$$\langle \mathcal{X}_{\text{CHSH}}\rangle \leqslant 2 + \varepsilon_{AB} + \varepsilon_{CB} + \varepsilon_{CD} + \varepsilon_{AD} \qquad (34)$$

holds. A violation of it implies that, in a possible HV model, certain conditional probability distributions have to be fundamentally different from experimentally preparable distributions.

Again, this result deserves some comments. First, note that the tested bound in Eq. (32) does not have to hold for all probability distributions in the theory. In an experiment testing Eq. (34) with some $\hat{p}_{\text{expt}}(\lambda)$, only assumptions about four conditional probability distributions (corresponding to two possible second measurements with two outcomes) have to be made. In fact, assuming Eq. (32) for $\delta$ distributions (i.e., a fixed HV $\lambda$) is not very physical, as in this case the left-hand side of these equations is 0 or 1.

Second, finding an experimental violation of Eq. (34) shows that these four distributions have properties significantly different from all preparable $p_{\text{expt}}(\lambda)$. In other words, one may conclude that in a possible HV model describing such an experiment, it must be forbidden to prepare $\hat{p}_{\text{expt}}(\lambda)$ with additional information about the result of $B$ or $D$.

To make this last point more clear, consider the situation where the experimenter has prepared $\hat{p}_{\text{expt}}(\lambda)$ and a second physicist has the additional knowledge that the result of $B_1$ will be $+1$ if it were measured as a first instance. Both physicists disagree on the probability distribution $\hat{p}_{\text{expt}}$ and $q^+$, but that is not the central problem because this occurs in any classical model as well. The point is that $q^+$ cannot be prepared: If the experimenter measures $B_1$ and keeps only the cases where he finds $+1$, he obtains a new experimentally accessible probability distribution $\tilde{p}_{\text{expt}}$. However, this will not be the same as the probability distribution $q^+$, because in this case, the first measurement has already been made.

### E. Application to the KCBS inequality and the KS inequality (15)

In the previous discussion, we used the CHSH-like inequality (7) to develop our ideas. Clearly, one could also start from inequalities (13) and (15) to obtain testable inequalities for the types of HV models discussed earlier in this article.

For the KCBS inequality (12) this can be done with the same methods as before, since the KCBS inequality uses only sequences of two measurements, as does the CHSH inequality (7). A generalization of Eq. (34) is

$$\langle \mathcal{X}_{\text{KCBS}}\rangle := \langle A_1 B_2\rangle + \langle C_1 B_2\rangle + \langle C_1 D_2\rangle + \langle E_1 D_2\rangle + \langle E_1 A_2\rangle$$
$$\geqslant -3 - (\varepsilon_{AB} + \varepsilon_{CB} + \varepsilon_{CD} + \varepsilon_{ED} + \varepsilon_{EA}). \qquad (35)$$

Generalizations of Eqs. (25) and (30) can also be written in a similar manner.

Also for the KS inequality (15), one can deduce generalizations, which exclude certain types of HV models. The main problem here is to estimate a term like $\langle A_1 B_2 C_3\rangle$. First, an inequality corresponding to Eq. (18) is

$$p[(A_1^+|A_1) \text{ and } (B_1^+|B_1) \text{ and } (C_1^+|C_1)]$$
$$\leqslant p[A_1^+, B_2^+, C_3^+|A_1 B_2 C_3]$$
$$+ p[(B_1^+|B_1) \text{ and } (B_2^-|A_1 B_2)]$$
$$+ p[(C_1^+|C_1) \text{ and } (C_3^-|A_1 B_2 C_3)], \qquad (36)$$

which holds again for any HV model. Then, a direct calculation gives that one has

$$\langle ABC\rangle \leqslant \langle A_1 B_2 C_3\rangle + 4p^{\text{flip}}[AB] + 4p^{\text{flip}}[(AB)C],$$
$$\langle ABC\rangle \geqslant \langle A_1 B_2 C_3\rangle - 4p^{\text{flip}}[AB] - 4p^{\text{flip}}[(AB)C], \qquad (37)$$

where

$$p^{\text{flip}}[(AB)C] = p[(C_1^+|C_1) \text{ and } (C_3^-|A_1B_2C_3)]$$
$$+ p[(C_1^-|C_1) \text{ and } (C_3^+|A_1B_2C_3)]. \quad (38)$$

Given these bounds, one arrives at testable inequalities, provided assumptions on the HV model are made as in the three approaches above. If Eq. (23) is assumed, one can directly estimate $p^{\text{flip}}[AB] \leqslant p^{\text{err}}[A_1B_2]$ and

$$p^{\text{flip}}[(AB)C] \leqslant p^{\text{err}}[(AB)C]$$
$$= p[C_1^+C_4^-|C_1A_2B_3C_4] + p[C_1^-C_4^+|C_1A_2B_3C_4]. \quad (39)$$

Then, if one writes the generalized form of Eq. (15), then there are more correction terms than in Eq. (25). Moreover, they involve sequences of length 4. On average, these $p^{\text{err}}$ terms have to be smaller than $2/48 \approx 0.0417$ in order to allow a violation. Consequently, an experimental test is very demanding (see also the discussion in Sec. IV C). Finally, generalizations in the sense of Eqs. (30) and (34) can also be derived in a similar manner.

## IV. EXPERIMENTAL IMPLEMENTATION

Experimental tests of noncontextual HV theories have been carried out with photons [35–38,46], neutrons [37,38], laser-cooled trapped ions [45], and liquid-state nuclear magnetic resonance systems [48]. In the experiments with photons and neutrons, single particles were prepared and measured in a four-dimensional state space composed of two two-dimensional state spaces describing the particle's polarization and the path it was following. In contrast, in a recent experiment with trapped ions [45], a composite system composed of two trapped ions prepared in superpositions of two long-lived internal states was used for testing the KS theorem. In the following, we will describe this experiment and present details about the amount of noncompatibility of the observables implemented.

### A. Experimental methods

Trapped laser-cooled ions are advantageous for these kinds of measurements because of the highly efficient quantum-state preparation and measurement procedures trapped ions offer. In Ref. [45], a pair of $^{40}\text{Ca}^+$ ions was prepared in a state space spanned by the states $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|00\rangle$, where $|1\rangle = |S_{1/2}, m_S = 1/2\rangle$ is encoded in a Zeeman ground state and $|0\rangle = |D_{5/2}, m_D = 3/2\rangle$ in a long-lived metastable state of the ion (see Fig. 1).

A key element for both preparation and measurement are laser-induced unitary operations that allow for arbitrary transformations on the four-dimensional state space. For this, the entangling operation (Mølmer-Sørensen gate operation) $U^{\text{MS}}(\theta, \phi) = \exp(-i\frac{\theta}{2}\sigma_\phi \otimes \sigma_\phi)$, where $\sigma_\phi = \cos(\phi)\sigma_x + \sin(\phi)\sigma_y$ is realized by a bichromatic laser field off-resonantly coupling to transitions involving the ions' center-of-mass mode along the weakest axis of the trapping potential [54]. In addition, collective single-qubit gates $U(\theta, \phi) = \exp[-i\frac{\theta}{2}(\sigma_\phi \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_\phi)]$ are realized by resonantly coupling the states $|0\rangle$ and $|1\rangle$. Finally, the single-qubit gate $U_z(\theta) = \exp(-i\frac{\theta}{2}\sigma_z)$ is implemented using a strongly focused laser inducing a differential light-shift on
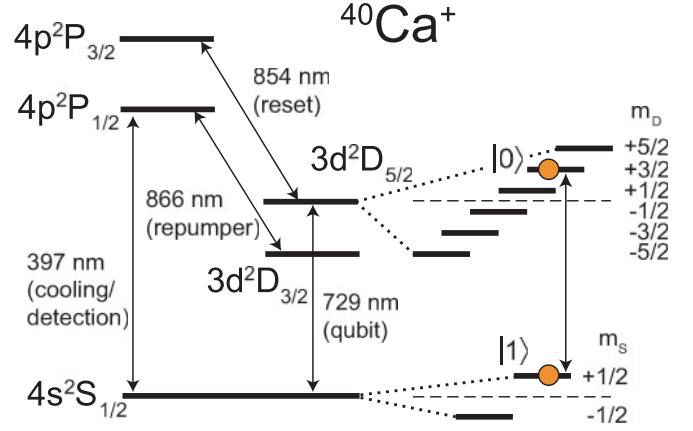


FIG. 1. (Color online) Partial level scheme of $^{40}\text{Ca}^+$ showing the relevant energy levels and the laser wavelengths needed for coupling the states. The $D$ states are metastable with a lifetime of about 1 s. A magnetic field of about 4 G is applied to lift the degeneracy of the Zeeman states. The states $|0\rangle$ and $|1\rangle$ used for encoding quantum information are indicated in the figure.

the states of the first ion. This set of operations, $\mathcal{S} = \{U_z(\theta), U(\theta, \phi), U^{\text{MS}}(\theta, \phi)\}$, which is sufficient for constructing arbitrary unitary operations, can be used for preparing the desired input states $|\psi\rangle$.

A measurement of $\sigma_z$ by a state projection onto the basis states $|0\rangle$ and $|1\rangle$ on one of the ions is carried out by illuminating the ion with laser light coupling the $S_{1/2}$ ground state to the short-lived excited state $P_{1/2}$ and detecting the fluorescence emitted by the ion with a photomultiplier. Population in $P_{1/2}$ decays back to $S_{1/2}$ within a few nanoseconds so that thousands of photons are scattered within a millisecond if the ion was originally in the state $|1\rangle$. If it is in state $|0\rangle$, it does not couple to the light field and therefore scatters no photons. In the experiment, we assign the state $|1\rangle$ to the ion if more than one photon is registered during a photon collection period of 250 $\mu$s. In this way, the observables $\sigma_z \otimes \mathbb{1}$ and $\mathbb{1} \otimes \sigma_z$ can be measured.

To measure further observables like $\sigma_i \otimes \mathbb{1}$, $\mathbb{1} \otimes \sigma_j$, or $\sigma_i \otimes \sigma_j$, the quantum state $\rho$ to be measured is transformed into $U\rho U^\dagger$ by a suitable unitary transformation $U$ prior to the state detection. Measuring the value of $\sigma_z \otimes \mathbb{1}$ on the transformed state is equivalent to measuring the observable $A = U^\dagger(\sigma_z \otimes \mathbb{1})U$ on the original state $\rho$. The measurement is completed by applying the inverse operation $U^\dagger$ after the fluorescence measurement. The purpose of this last step is to map the projected state onto an eigenstate of the observable $A$. In this way, any observable $A$ with two pairs of degenerate eigenvalues can be measured. The complete measurement, consisting of unitary transformation, fluorescence detection, and back transformation, constitutes a quantum nondemolition measurement of $A$. Each measurement of a quantum state yields one bit of information which carries no information about other compatible observables.

### B. Measurement results

The measurement procedure outlined in the preceding section is very flexible and can be used to consecutively measure several observables on a single quantum system,
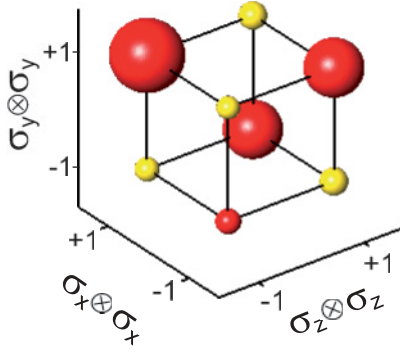
FIG. 2. (Color online) Measurement correlations for a sequence of measurements $A_1 B_2 C_3$ with $A_1 = \sigma_z \otimes \sigma_z$, $B_2 = \sigma_x \otimes \sigma_x$, and $C_3 = \sigma_y \otimes \sigma_y$ for a partially entangled input state. The colors indicate whether $v_1 v_2 v_3 = +1$ [yellow (light gray) spheres] or $v_1 v_2 v_3 = -1$ [red (dark gray) spheres]. The volume of a sphere is proportional to the likelihood of finding the corresponding measurement outcome $(v_1, v_2, v_3)$.

as illustrated by the following example. To test inequality Eq. (14) for the observables of the Mermin-Peres square (16), the quantum state $|\psi\rangle = |11\rangle/\sqrt{2} + e^{i\frac{\pi}{4}}(|01\rangle + |10\rangle)/2$ is prepared by a applying the sequence of gates $U^{\mathrm{MS}}(-\pi/2, \pi/4)U^{\mathrm{MS}}(-\pi/2, 0)U(\pi/2, 0)$ to the initial state $|11\rangle$. The correlations that are found for a sequence of measurements $A_1 B_2 C_3$, where $A_1 = \sigma_z \otimes \sigma_z$, $B_2 = \sigma_x \otimes \sigma_x$, and $C_3 = \sigma_y \otimes \sigma_y$, are shown in Fig. 2. For this measurement, 1100 copies of the state were created and measured. Each corner of the sphere corresponds to a measurement outcome $(v_1, v_2, v_3)$ where $v_k = \pm 1$ is the measurement result for the $k$th observable. The relative frequencies of the measurement outcomes are indicated by the volume of the spheres attached to the corners, and the colors indicate whether $v_1 v_2 v_3 = +1$ or $v_1 v_2 v_3 = -1$. For perfect state preparation and measurements, one would expect to observe always $v_1 v_2 v_3 = -1$. Due to experimental imperfections, the experiment yields $\langle v_1 v_2 v_3 \rangle = -0.84(2)$. Nevertheless, the experimental results nicely illustrate the quantum measurement process: the first measurement gives $\langle \sigma_z \otimes \sigma_z \rangle = 0.00(2)$; that is, the state $|\psi\rangle$ is equally likely to be projected onto $|\Psi_+\rangle = |11\rangle$ $(v_1 = +1)$ and onto $|\Psi_-\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$ $(v_1 = -1)$. In the latter case, the projected state $|\Psi_-\rangle$ is an eigenstate of $\sigma_x \otimes \sigma_x$ and $\sigma_y \otimes \sigma_y$ so that these measurements give definite results $v_2 = +1$ and $v_3 = +1$ (top left corner of Fig. 2). In the former case, the projected state is not an eigenstate of $\sigma_x \otimes \sigma_x$ and $v_2 = +1$ and $v_3 = -1$ are found with equal likelihood. In this case, $v_2$ and $v_3$ are random but correlated with $v_2 v_3 = 1$ (the other two strongly populated corners of Fig. 2).

In Ref. [45], also the other rows and columns of the Mermin-Peres square (16) were measured for the state $|\psi\rangle$, and a violation of Eq. (14) was found with $\langle \chi_{\mathrm{KS}} \rangle = 5.36(4)$. Also, different input states were investigated to check that the violation is indeed state-independent. The fact that the result falls short of the quantum-mechanical prediction of $\langle \chi_{\mathrm{KS}} \rangle = 6$ is due to imperfections in the measurement procedure. These imperfections could be incorrect unitary transformations but could also be errors occurring during the fluorescence measurement.

TABLE I. Measurement correlations $\langle A_i A_j | A_1 \cdots A_5 \rangle$ between repeated measurements of $A = \sigma_z \otimes \mathbb{1}$ for a maximally mixed state. Observing a correlation of $\langle A_i A_j | A_1 \cdots A_5 \rangle = \alpha_{ij}$ means that the probability of the measurement results of $A_i$ and $A_j$ coinciding equals $(\alpha_{ij} + 1)/2$.

| Measurement | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| 1 | 0.97(1) | 0.97(1) | 0.96(1) | 0.95(1) |
| 2 | | 0.97(1) | 0.97(1) | 0.96(1) |
| 3 | | | 0.98(1) | 0.98(1) |
| 4 | | | | 0.98(1) |

An instructive test consists of repeatedly measuring the same observable on a single quantum system and analyzing the measurement correlations. Table I shows the results of five consecutive measurements of $A = \sigma_z \otimes \mathbb{1}$ on a maximally mixed state based on 1100 experimental repetitions.

As expected, the correlations $\langle A_i A_{i+k} | A_1 \cdots A_5 \rangle$ are independent of the measurement number $i$ within the error bars. However, the correlations become smaller and smaller the bigger $k$ gets. Table II shows another set of measurement correlations $\langle A_i A_j | A_1 \cdots A_5 \rangle$, where $A = \sigma_x \otimes \sigma_x$. Here, the correlations are slightly smaller, since entangling interactions are needed for mapping $A$ onto $\sigma_z \otimes \mathbb{1}$, which is experimentally the most demanding step.

It is also interesting to compare the correlations $\langle A_1 A_3 | A_1 A_2 A_3 \rangle$ with the correlations $\langle A_1 A_3 | A_1 B_2 A_3 \rangle$ for an observable $B$ that is compatible with $A$. For $A = \sigma_x \otimes \sigma_x$ and $B = \sigma_z \otimes \sigma_z$, we find $\langle A_1 A_3 | A_1 A_2 A_3 \rangle = 0.88(1)$ and $\langle A_1 A_3 | A_1 B_2 A_3 \rangle = 0.83(2)$ when measuring a maximally mixed state; that is, it seems that the intermediate measurement of $B$ perturbs the correlations slightly more than an intermediate measurement of $A$. Similar results are found for a singlet state, where $\langle A_1 A_3 | A_1 A_2 A_3 \rangle = 0.92(1)$ and $\langle B_1 B_3 | B_1 B_2 B_3 \rangle = 0.91(1)$, but $\langle A_1 A_3 | A_1 B_2 A_3 \rangle = 0.90(1)$ and $\langle B_1 B_3 | B_1 A_2 B_3 \rangle = 0.89(1)$. Because $\langle B_1 B_3 | B_1 A_2 B_3 \rangle = 1 - 2p^{\mathrm{err}}(B_1 A_2 B_3)$, correlations of the type $\langle B_1 B_3 | B_1 A_2 B_3 \rangle$ are required for checking inequality (25) that takes into account disturbed HVs.

### C. Experimental limitations

There are a number of error sources contributing to imperfect state correlations, the most important being the following.

TABLE II. Measurement correlations $\langle A_i A_j | A_1 \cdots A_5 \rangle$ between repeated measurements of $A = \sigma_x \otimes \sigma_x$ for a maximally mixed state. Observing a correlation of $\langle A_i A_j | A_1 \cdots A_5 \rangle = \alpha_{ij}$ means that the probability of the measurement results of $A_i$ and $A_j$ coinciding equals $(\alpha_{ij} + 1)/2$.

| Measurement | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| 1 | 0.94(1) | 0.88(1) | 0.82(2) | 0.80(2) |
| 2 | | 0.93(1) | 0.87(2) | 0.84(2) |
| 3 | | | 0.90(1) | 0.87(2) |
| 4 | | | | 0.93(1) |

### *1. Wrong state assignment based on fluorescence data*

During the $250$-$\mu$s detection period of the current experiment, the number of detected photons has a Poissonian distribution with an average number of $\bar{n}_{|1\rangle} = 8$ photons if the ion is in state $|1\rangle$. If the ion is in state $|0\rangle$, it does not scatter any light; however, light scattered from trap electrodes gives rise to a Poissonian distribution with an average number of $\bar{n}_{|0\rangle} = 0.08$ photons. These photon count distributions slightly overlap. The probability of detecting 0 or 1 photons even though the ion is in the bright state is 0.3%. The probability of detecting more than 1 photon if the ion is in the dark state is also 0.3%. Therefore, if the threshold for discriminating between the dark and the bright state is set between 1 and 2, the probability for wrongly assigning the quantum state is 0.3%. Making the detection period longer would reduce this error but increase errors related to decoherence of the other ion's quantum state that is not measured.

### *2. Imperfect optical pumping*

During fluorescence detection, the ion leaves the computational subspace $\{|0\rangle, |1\rangle\}$ if it was in state $|1\rangle$ and can also populate the state $|S_{1/2}, m_S = -1/2\rangle$. To prevent this leakage, the ion is briefly pumped on the $S_{1/2} \leftrightarrow P_{1/2}$ transition with $\sigma_+$-circularly polarized light to pump the population back to $|1\rangle$. Due to imperfectly set polarization and misalignment of the pumping beam with the quantization axis, this pumping step fails with a probability of about 0.5%.

### *3. Interactions with the environment*

Due to the nonzero differential Zeeman shift of the states used for storing quantum information, superposition states dephase in the presence of slowly fluctuating magnetic fields. In particular, while measuring one ion using fluorescence detection, quantum information stored in the other ion dephases. We partially compensate for this effect with spin-echo-like techniques [55] that are based on a transient storage of superposition states in a pair of states having an opposite differential Zeeman shift as compared to the states $|0\rangle$ and $|1\rangle$. A second interaction to be taken into account is spontaneous decay of the metastable state $|0\rangle$, which, however, only contributes an error of smaller than 0.1%.

### *4. Imperfect unitary operations*

The mapping operations are not error-free. This concerns in particular the entangling gate operations needed for mapping the eigenstate subspace of a spin correlation $\sigma_i \otimes \sigma_j$ onto the corresponding subspaces of $\sigma_z \otimes \mathbb{1}$. For this purpose, a Mølmer-Sørensen gate operation $U^{\mathrm{MS}}(\pi/2, \phi)$ [54,56] is used. This gate operation has the crucial property of requiring the ions only to be cooled into the Lamb-Dicke regime. In the experiments, the center-of-mass mode used for mediating the gate interaction is in a thermal state with an average of 18 vibrational quanta. In this regime, the gate operation is capable of mapping $|11\rangle$ onto a state $|00\rangle + e^{i\phi}|11\rangle$ with a fidelity of about 98%. Taking this fidelity as being indicative of the gate fidelity, one might expect errors of about 4% in each measurement of spin correlations $\sigma_i \otimes \sigma_j$ as the gate is

carried out twice, once before and once after the fluorescence measurement.

These error sources prevented us from testing a generalization of inequality (15), as discussed in Sec. III E. Measurement of the correlations $\langle B_1 B_3 | B_1 A_2 B_3 \rangle$ and $\langle C_1 C_4 | C_1 A_2 B_3 C_4 \rangle$ resulted in error terms $p^{\mathrm{err}}$ that were about 0.06 for sequences involving three measurements and about 0.1 for sequences with four measurements, that is, twice as big as required for observing a violation of (15). However, the experimental errors were small enough to demonstrate a violation of the CHSH-like inequality (25), valid for nonperfectly compatible observables [45]. A test of the inequality (30) would become possible if the error rates could be further reduced.

## V. CONTEXTUAL HV MODELS

In this section we will introduce two HV models which are contextual in the sense of Eq. (3) and violate the inequalities discussed in Sec. II. We first discuss a simple model which violates inequality (25) and then a more complex one which reproduces all measurement results for a (finite-dimensional) quantum-mechanical system. These models are useful for pointing out which counterintuitive properties a HV model must have to reproduce the quantum predictions and which further experiments can rule out even these models.

### A. A simple HV model leading to a violation of inequality (25)

We will show here that violation of inequality (25) can be achieved simply by allowing the HV model to remember what measurements have been performed and what the outcome was. The basic idea of the model is very simple (cf. the more complicated presentation in [49]).

The task is to construct a simple HV model for our four dichotomic observables $A$, $B$, $C$, and $D$. The HV $\lambda$ is taken to be a quadruple with entries taken from the set $\{+, -, \oplus, \ominus\}$; the latter two cases will be called "locked" in what follows, signifying that the value is unchanged whenever a compatible measurement is made. For convenience, we can write $\lambda = (A^+, B^+, C^+, D^+)$ or $\lambda = (A^+, B^-, C^\oplus, D^\ominus)$, etc., and we take the initial distribution to be probability $1/2$ of either $(A^+, B^+, C^+, D^+)$ or $(A^-, B^-, C^-, D^-)$. The measurement of an observable is simply reporting the appropriate sign and locking the value in the position. To make the model contextual, we add the following mechanism:

(a) If $A$ is measured, then the sign of $D$ is reversed and locked unless it is locked.
(b) If $D$ is measured, then the sign of $A$ is reversed and locked unless it is locked.

For the case $\lambda = (A^+, B^+, C^+, D^+)$, the measurement results when measuring inequality (25) will be as follows.

(i) Measurement of $A_1$ will yield $A_1^+$ and $\lambda = (A^\oplus, B^+, C^+, D^\ominus)$, and for the next measurement one obtains $B_2^+$ or $D_2^-$.
(ii) Measurement of $B_1$ will yield $B_1^+$ and $\lambda = (A^+, B^\oplus, C^+, D^+)$, and further one obtains $A_2^+ B_3^+$ or $C_2^+ B_3^+$.

(iii) Measurement of $C_1$ will yield $C_1^+$ and $\lambda = (A^+, B^+, C^\oplus, D^+)$, and we will obtain $B_2^+$ or $D_2^+$ afterward.

(iv) Measurement of $D_1$ will yield $D_1^+$ and $\lambda = (A^\ominus, B^+, C^+, D^\oplus)$, and we will obtain $C_2^+ D_3^+$ or $A_2^- D_3^+$. The latter is because a measurement of $A_2$ will not change $D^\oplus$ since it is locked. In this case, after a measurement of $A_2$, the HVs are $\lambda = (A^\ominus, B^+, C^+, D^\oplus)$.

The case $\lambda = (A^-, B^-, C^-, D^-)$ is the same with reversed signs. This means that

$$\langle A_1 B_2 \rangle = \langle C_1 B_2 \rangle = \langle C_1 D_2 \rangle = -\langle A_1 D_2 \rangle = 1, \quad (40)$$

and

$$
\begin{aligned}
p^{\mathrm{err}}[B_1 A_2 B_3] &= p^{\mathrm{err}}[B_1 C_2 B_3] = p^{\mathrm{err}}[D_1 C_2 D_3] \\
&= p^{\mathrm{err}}[D_1 A_2 D_3] = 0.
\end{aligned}
\quad (41)
$$

Hence, this model leads to the maximal violation of Eq. (25).

In this model, the observables $A$ and $D$ are compatible in the sense of Definition 1, but they maximally violate the noncontextuality condition in Eq. (3). It is easy to verify that $p^{\mathrm{flip}}[AD] = 1$, so that assumption (23) does not hold. We argue that in this model, the change in the outcome $D$ cannot be explained as merely due to a disturbance of the system from the experimental procedures when measuring $A_1$. It should therefore be no surprise that the inequality (25) is violated by the model. Finally, note that a model behavior like this would create problems in any argument to establish noncontextuality via repeatability of compatible measurements, even for joint measurements as discussed in Sec. II A, and not only in the sequential setting used here.

### B. A HV model explaining all quantum-mechanical predictions

Let us now introduce a detailed HV model which reproduces all the quantum predictions for sequences of measurements. In a nutshell, this contextual HV model is a translation of a machine that classically simulates a quantum system.

We consider the case in which only dichotomic measurements are performed on the quantum-mechanical system. Therefore, any observable $A$ decomposes into $A = \Pi_+^A - \Pi_-^A$ with orthogonal projectors $\Pi_+$ and $\Pi_-$. For a mixed state $\varrho$, a measurement of this observable produces the result $+1$ with probability $p(A^+) = \mathrm{tr}(\Pi_+^A \rho)$ and the result $-1$ with probability $p(A^-) = \mathrm{tr}(\Pi_-^A \rho)$. In addition, the measurement apparatus will modify the quantum state according to

$$\varrho \mapsto \frac{\Pi_\pm^A \varrho \Pi_\pm^A}{\mathrm{tr}(\Pi_\pm^A \varrho)}, \quad (42)$$

depending on the measurement result $\pm 1$.

This behavior can be exactly mimicked by a HV model if we allow the value of the HV to be modified by the action of the measurement. If $\mathcal{H}$ is the Hilbert space of the quantum system, we use two types of HV. First, we use parameters $0 \leqslant \lambda^A < 1$, $0 \leqslant \lambda^B < 1$, etc., for each observable $A$, $B$, etc., and second, we use a normalized vector $|\psi\rangle \in \mathcal{H}$.

Then, for given values of all these parameters, we associate to any observable the measurement result as follows: We define $q^A = \langle \psi | \Pi_-^A | \psi \rangle$ and let the model predict the measurement

result: $-1$ if $\lambda^A < q^A$ and $+1$ if $q^A \leqslant \lambda^A$. Furthermore, depending on the measurement result, the values of the HVs $\lambda^A$ and $|\psi\rangle$ change according to

$$
\lambda^A \mapsto
\begin{cases}
\dfrac{\lambda^A}{q^A} & \text{if } \lambda^A < q^A, \\[2mm]
\dfrac{\lambda^A - q^A}{1 - q^A} & \text{if } \lambda^A \geqslant q^A,
\end{cases}
\quad (43)
$$

and

$$
|\psi\rangle \mapsto
\begin{cases}
\dfrac{\Pi_-^A |\psi\rangle}{\sqrt{q^A}} & \text{if } \lambda^A < q^A, \\[2mm]
\dfrac{\Pi_+^A |\psi\rangle}{\sqrt{1 - q^A}} & \text{if } \lambda^A \geqslant q^A.
\end{cases}
\quad (44)
$$

Let us now fix the initial probability distribution of the HVs. The experimentally accessible probability distributions $p(\lambda^A, \lambda^B, \ldots; \psi)$ shall not depend on the parameters $\lambda^A, \lambda^B, \ldots$; that is, $p(\lambda^A, \lambda^B, \ldots; \psi) = p(\lambda'^A, \lambda'^B, \ldots; \psi)$. Hence, we write $p(\psi) = \int d\lambda^A d\lambda^B \cdots p(\lambda^A, \ldots; \psi)$. The probability distribution $p(\psi)$ and the measure $d\psi$ are chosen such that

$$\varrho_p = \int d\psi \ p(\psi) |\psi\rangle\langle\psi| \quad (45)$$

is the corresponding quantum state.

We now verify that this model indeed reproduces the quantum predictions. If the initial distribution is $p$, then the probability of obtaining the result $-1$ for $A$ is given by

$$
\begin{aligned}
p_-^A &= \int_{\lambda^A < q^A} d\lambda^A d\psi \ p(\psi) = \int d\psi \ \langle \psi | \Pi_-^A | \psi \rangle p(\psi) \\
&= \mathrm{tr}(\rho_p \Pi_-^A)
\end{aligned}
\quad (46)
$$

and hence is in agreement with the quantum prediction. Due to the transformations in Eqs. (43) and (44), the probability distribution changes by the action of the measurement, $p \mapsto p'$. The new distribution $p'$ again does not depend on $\lambda^A$ and, in the case of the measurement result $-1$, we have

$$p'(\psi) = \frac{1}{p_-^A} \int d\psi' q'^A \ \delta\left(|\psi\rangle - \frac{\Pi_-^A |\psi'\rangle}{\sqrt{q'^A}}\right) p(\psi'), \quad (47)$$

where $\delta$ denotes Dirac's $\delta$ distribution and $q'^A = \langle \psi' | \Pi_-^A | \psi' \rangle$. The new corresponding mixed state is given by

$$
\begin{aligned}
\varrho_{p'} &= \int d\psi \ p'(\psi) |\psi\rangle\langle\psi| \\
&= \frac{1}{p_-^A} \int d\psi' \ p(\psi') \Pi_-^A |\psi'\rangle\langle\psi'| \Pi_-^A \\
&= \frac{\Pi_-^A \varrho_p \Pi_-^A}{\mathrm{tr}(\varrho_p \Pi_-^A)}.
\end{aligned}
\quad (48)
$$

This demonstrates that the transformation in Eq. (42) is suitably reproduced by $\varrho_p \mapsto \varrho_{p'}$. An analogous calculation can be performed for the measurement result $+1$.

Let us illustrate that this model is actually contextual, as defined in Eq. (3). As an example, we choose two commuting observables $A = \Pi_+^A - \Pi_-^A$ and $B = \Pi_+^B - \Pi_-^B$ with the property that, for some pure state $|\psi\rangle$, we have $\langle \psi | A_1 B_2 | \psi \rangle = +1$,

while $\langle\psi|B|\psi\rangle < 1$. An example would be $A = \sigma_z \otimes \mathbb{1}$ and $B = -\mathbb{1} \otimes \sigma_z$ with $|\psi\rangle$ being the singlet state. Then, after a measurement of $A_1$, the result of a subsequent measurement of $B_2$ is fixed and hence independent of $\lambda^B$. However, if $B$ is measured without a preceding measurement of $A$, then the result of $B$ will be $-1$ if $\lambda^B < \langle\psi|\Pi_-^B|\psi\rangle$ and $+1$ otherwise. Hence, in our particular model, given the preparation of $|\psi\rangle$, $v(B_1)$ depends on $\lambda^B$, while $v(B_2|A_1 B_2)$ only depends on $\lambda^A$. However, the model does not allow special correlations between $\lambda^A$ and $\lambda^B$ and hence the model is contextual; that is, necessarily, there are experimentally accessible values of the HVs such that Eq. (3) is violated.

## VI. CONCLUSIONS

Experimental quantum contextuality is a potential source of new applications in quantum information processing and a chance to expand our knowledge on the reasons why quantum resources outperform classical ones. In some sense, experimental quantum contextuality is an old discipline, since most Bell experiments are just experiments ruling out noncontextual HV models, since they do not fulfill the required spacelike separation needed to invoke locality as a physical motivation behind the assumption of noncontextuality. The possibility of observing state-independent quantum contextuality, however, is a recent development. It shows that the power of QM is not necessarily in some particular states, but also in some sets of measurements which can reveal nonclassical behavior of any quantum state.

These experiments must satisfy some requirements which are not explicitly needed for tests of Bell inequalities. An important requirement is that one has to test experimentally to what extent the implemented measurements are indeed compatible. In this article, we have discussed how to deal with the inevitable errors preventing researchers from implementing perfectly compatible measurements. The problem of imperfectly compatible observables is not fatal, but should be taken into account with care.

We have presented three approaches by which additional requirements can be used to exclude the possibility of noncontextual explanations of the experimental results, and we have applied them to three specific inequalities of particular interest: a CHSH-like noncontextuality inequality using sequential measurements on individual systems, which can be violated by specific states of four or more levels; a KCBS noncontextuality inequality using sequential measurements on individual systems, which can be violated by specific states of three or more levels; and a KS inequality coming from the Mermin-Peres square, which is violated by any state of a four-level system. Similar methods can be applied to any noncontextuality inequality, irrespective of the number of sequential measurements or the dimensionality of the Hilbert space.

The main motivation was to provide experimentalists with inequalities to rule out noncontextual HV models unambiguously if some additional assumptions are made. We have shown that a recent experiment with trapped ions already ruled out some of these HV models. By providing examples of HV models, we have seen that these extra assumptions are not necessarily satisfied by very artificial HV models.

Nevertheless, they lead to natural extensions of the assumption of noncontextuality and allow us to reach conclusions about HV models in realistic experiments with nonperfect devices. An interesting line of future research will be to investigate how these extra assumptions can be replaced by fundamental physical principles such as locality in experiments where the system under observation is entangled with a distant system on which additional measurements can be performed.

## APPENDIX

In Sec. II C we discussed the notion of compatibility for subsequent measurements. In this appendix we provide two examples which demonstrate that both parts of Definition 1 are independent. We then show that the statement of compatibility can be simplified to involve sequences of length 2 only.

### A. Mutual independence of Definition 1 (i) and Definition 1 (ii)

For an example in which (i) does not include (ii), assume that the expectation value of $A$ depends on whether the first measurement in the sequence is $A$ or $B$. Then $\langle A_1|A_1 B_2\rangle \neq \langle A_2|B_1 A_2\rangle$ and hence condition (ii) is violated. However, such a model is not in conflict with condition (i) if, once $A$ was measured, the value of $A$ stays unchanged for the rest of the sequence.

For the converse, assume a HV model where the expected value $\langle A\rangle$ does not depend on the results of any previous measurement. Then, for any sequence and any $k$, $\langle A\rangle = \langle A_k|S\rangle$ and, hence, condition (ii) is satisfied. However, $p(A_1^+ A_2^-|A_2 A_2) > 0$, unless $\langle A_1 A_2\rangle = 1$, and thus condition (i) is violated.

### B. Compatibility for sequences of length 2

Assume that, for any preparation procedure, $A$ and $B$ obey

$$\langle A_1\rangle = \langle A_2|A_1 A_2\rangle = \langle A_2|B_1 A_2\rangle; \tag{A1}$$

that is, condition (ii) of Definition 1 is satisfied for sequences of length 2. Then, for a sequence $S$ of length $k$ we have either $S = S'B$ or $S = S'A$, where $S'$ is a sequence of length $k-1$. In a measurement of $S$, we can consider $S'$ to be part of the preparation procedure and then apply Eq. (A1). It follows that $\langle A_{k+1}|SA\rangle = \langle A_k|S'A\rangle$ and eventually $\langle A_{k+1}|SA\rangle = \langle A_1\rangle$ by induction.

In a similar fashion we reduce condition (i) of Definition 1 for dichotomic observables. For an experimentally accessible probability distribution $p_{\text{expt}}(\lambda)$, we denote by $\tilde{p}_{\text{expt}}(\lambda)$ the

distribution obtained by a measurement of $A$ and a post-selection of the result $+1$. Then, for a sequence $S$ of length $k$,

$$p(A_1^+ A_{k+2}^- | ASA) = \tilde{p}(A_{k+1}^- | SA) p(A_1^+ | A_1)$$
$$= \tilde{p}(A_1^- | A) p(A_1^+ | A)$$
$$= p(A_1^+ A_2^- | A_1 A_2), \qquad \text{(A2)}$$

where for the second equality we used that $\langle A_{k+1} | SA \rangle = \langle A_1 \rangle$ holds for $\tilde{p}$. It follows that a set of dichotomic observables $\Xi$ is compatible if and only if, for any preparation and any $A, B \in \Xi$, $\langle A_1 A_2 \rangle = 1$ and Eq. (A1) holds. In particular, this proves the assertion that pairwise compatibility of three or more observables is equivalent to an extended definition of compatibility involving sequences of all compatible observables.

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