Invertible Map between Bell Nonlocal and Contextuality Scenarios

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We present an invertible map between correlations in any bipartite Bell scenario and behaviors in a family of contextuality scenarios. The map takes local, quantum, and no-signaling correlations to noncontextual, quantum, and contextual behaviors, respectively. Consequently, we find that the membership problem of the set of quantum contextual behaviors is undecidable, the set cannot be fully realized via finite dimensional quantum systems and is not closed. Finally, we show that neither this set nor its closure is the limit of a sequence of computable supersets due to the result $\mathrm{MIP}^* = \mathrm{RE}$.

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Introduction.—Bell nonlocality [1] describes correlations between spacelike separated experiments that are impossible in any locally realistic theory. Such correlations are, however, allowed in quantum theory. Beyond their fundamental relevance these correlations have technological applications such as secure random number generation [2] and cryptography [3].

Generalized contextuality [4] similarly describes correlations that are absent from classical physics but instead of spacelike separation, these correlations occur in experiments where there are *operationally equivalent* experimental procedures. For example, two preparation procedures of a system are operationally equivalent if every measurement on the system leads to the same statistics for both preparation procedures. Contextual correlations have also found practical relevance, for example, in state discrimination [5] and demonstrating quantum advantage in communication tasks [6].

One way to enforce an operational equivalence between preparations is by using the setup of a Bell nonlocality experiment (known as a Bell scenario), under the assumption that no signal can travel faster than light. In a two-party Bell scenario two parties, Alice and Bob, share a physical system. In some frame of reference, Alice selects and performs a measurement x from some pre-agreed options on her subsystem, then Bob measures his subsystem at a time before any light signal could have arrived.

Under the no-signaling assumption, the statistics Bob can observe from such a measurement must not depend on x, otherwise by performing this procedure with many shared systems simultaneously Bob could infer Alice's choice x and a faster-than-light signal could be transmitted from Alice to Bob. It follows that viewing Alice's measurement of her subsystem as a preparation procedure for Bob's subsystem, the preparation of Bob's system given by a choice, x, of Alice must be operationally equivalent to that given by any other choice, x', of Alice. In this way, a Bell scenario is viewed as a *remote*-preparation and measurement experiment with preparation equivalences, and is therefore, an example of a contextuality scenario.

In this Letter we use this intuition to define a mapping between these scenarios and show that the set of quantum correlations in a given two-party Bell scenario is isomorphic to the union of the sets of quantum correlations in an indexed [7] family of contextuality scenarios [8] (see Fig. 1). The quantum Bell correlations we consider are those given by the tensor product formalism for potentially infinite dimensional quantum systems, denoted $\mathcal{C}_{\mathrm{qs}}$ for quantum spatial correlations. We further show that this mapping is also a bijection between the local (no-signaling) correlations and the noncontextual (contextual) correlations, respectively, in these scenarios.

The map and showing its theory-preserving nature form our first main contribution. Combining these results with the remote-preparation perspective shows that *if a physical theory predicts the generalized contextual correlations of quantum theory, then that theory is exactly limited to producing the quantum spatial correlations in any two-party Bell scenario, under the no-signaling assumption.* Thus, we demonstrate a characterization of the set of the quantum spatial correlations in terms of contextuality.

The connection between two-party Bell scenarios and (prepare-and-measure) contextuality scenarios is noted in various works [5,9,10]; see also [11]. In these works, the relationship is described via examples and the general case is not addressed, meaning the statement above was not established.

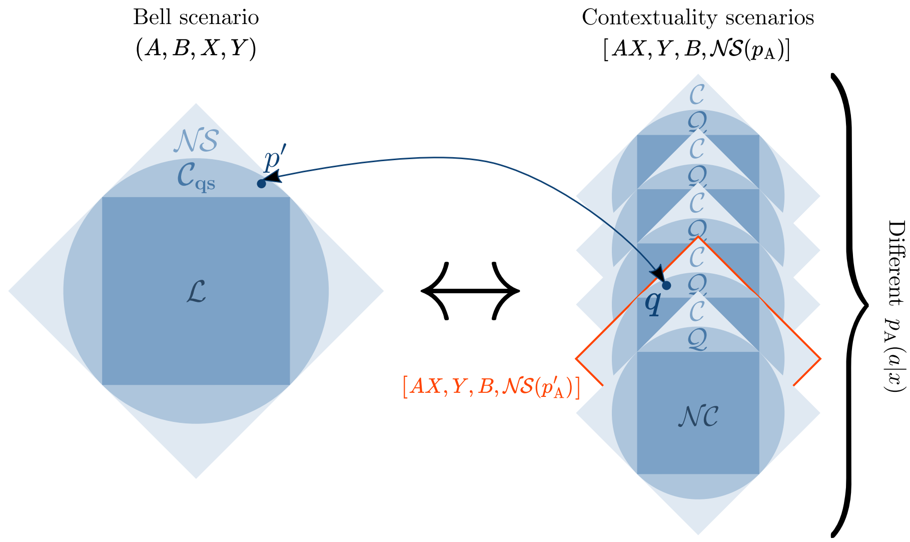

FIG. 1. A schematic representation of the invertible map between correlations in a Bell scenario and behaviors in a family of contextuality scenarios. Here, $\mathcal{L}$, $\mathcal{C}_{qs}$, and $\mathcal{NS}$ denote the local, quantum spatial, and no-signaling sets of correlations in Bell scenarios, while $\mathcal{NC}$, $\mathcal{Q}$, and $\mathcal{C}$ denote the noncontextual, quantum, and contextual sets of behaviors in contextuality scenarios (see the main text for more details).

Furthermore, it was previously thought that all contextuality scenarios of a certain kind (in which there are no measurement equivalences and the preparation equivalences comprise various decompositions of one single hypothetical preparation) could be mapped to Bell scenarios in this manner [[5], Sec. VII]. However, we find examples of such scenarios in which this mapping is not possible. Of course, this does not rule out an isomorphism in this case but a different map would be required.

In our second main contribution, we use our isomorphism to deduce various properties of the quantum set of contextual correlations, including membership undecidability, the necessity of infinite dimensional quantum systems in realizing all quantum correlations, and nonconvergence to the quantum set of semidefinite programming (SDP) hierarchies [15,16].

This final result follows from showing that a computable hierarchy of outer approximations converging to the quantum set of contextual correlations would give rise to an algorithm capable of deciding the weak membership problem for the closure $\mathcal{C}_{qa}$ of $\mathcal{C}_{qs}$. However, this problem is known to be undecidable as a consequence of the result $\mathrm{MIP}^* = \mathrm{RE}$ [17]. This result raises several open questions. To what superset, $\mathcal{Q}_\infty$, of quantum correlations do the SDP hierarchies in Refs. [15,16] converge? What would be the image of $\mathcal{Q}_\infty$ in the Bell setting under our mapping? A natural candidate could be the set of quantum commuting correlations, which generally maps to a strict superset of the quantum contextual correlations under our mapping. If this is the case, does $\mathcal{Q}_\infty$ have a physical interpretation in the contextuality setting? Alternatively, the image of $\mathcal{Q}_\infty$ might provide a new outer approximation of the set $\mathcal{C}_{qs}$.

In the main text we will describe our map for Bell correlations in which each of Alice's outcomes occurs with nonzero probability. This case encapsulates the central concepts of the map and avoids some technicalities of the general case. In the Supplemental Material [18] we provide a complete description of the map that is used to prove our main results.

Bell scenarios.—A *two-party Bell scenario* comprises two spacelike separated experiments. In the first, a party, call her Alice, selects an input from the set $[X] := \{1, \ldots, X\}$, for some $X \in \mathbb{N}$ and observes an outcome from a set $[A]$, for some $A \in \mathbb{N}$. In the second, another party, call him Bob, similarly selects an input from the set $[Y]$, for some $Y \in \mathbb{N}$ and observes an outcome from a set $[B]$, for some $B \in \mathbb{N}$. The specific scenario can therefore be identified by the tuple of four numbers (A, B, X, Y), indicating the numbers of inputs and outputs for each party. Unless otherwise stated, variables a, b, x, y take values from the sets $[A]$, $[B]$, $[X]$, $[Y]$ throughout.

Given a Bell scenario (A, B, X, Y), a correlation is given by a vector $p \in \mathbb{R}^{ABXY}$, with entries $p(a, b|x, y)$ that specify the probability of Alice and Bob observing outcomes a and b given inputs x and y, respectively. In this Letter, we will primarily consider the set $\mathcal{C}_{qs}$ of quantum correlations in a Bell scenario using the tensor product formulation and allowing for infinite dimensional quantum systems. A correlation, p, is in the quantum set, $\mathcal{C}_{qs}$, if

$$p(a, b|x, y) = \mathrm{Tr}(M_a^x \otimes N_b^y \rho), \tag{1}$$

for some positive-operator-valued measures (described in the finite-outcome case by a collection of positive semidefinite operators summing to the identity operator) $M^x = \{M_a^x\}_a$ and $N^y = \{N_b^y\}_b$ on a separable Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and a density operator (positive semidefinite operator with unit trace) ρ on $\mathcal{H}_A \otimes \mathcal{H}_B$.

A strict superset of the quantum set is the so-called *no-signaling* set, described by correlations p satisfying the no-signaling constraints

$$\sum_b p(a,b|x,y) = \sum_b p(a,b|x,y') \quad \forall\, a,x,y,y' \tag{2}$$

$$\sum_a p(a,b|x,y) = \sum_a p(a,b|x',y) \quad \forall\, b,y,x,x'. \tag{3}$$

A strict subset of the quantum set (considered "classical" in Bell scenarios) is the *local set*. A correlation, p, is local if there exists a measurable space (Λ, Σ), a probability measure $\mu\colon \Sigma \to [0,1]$, and local probability distributions $l^A(a|x,E)$ and $l^B(b|y,E)$ satisfying $\sum_a l^A(a|x,E) = \sum_b l^B(b|y,E) = 1$ for all x, y and nonempty $E \in \Sigma$, such that

$$p(a,b|x,y) = \int_\Lambda l^A(a|x,\lambda) l^B(b|y,\lambda) \mathrm{d}\mu(\lambda). \tag{4}$$

The relationship between the sets $\mathcal{L}$, $\mathcal{C}_{qs}$, and $\mathcal{NS}$ is depicted on the left-hand side of Fig. 1.

Contextuality scenarios.—A *contextuality scenario* is an experiment capable of revealing the impossibility of modeling a physical system with a noncontextual ontological model. A key concept in generalized contextuality is operational equivalence, so we will want operational equivalence to appear in our experiment. For our purposes operational equivalence between preparation procedures is sufficient.

Two preparation procedures, P_1 and P_2, for a system are operationally equivalent, denoted $P_1 \simeq P_2$, in a theory when any outcome of any measurement on the system would occur with the same probability whether the measurement is performed on a system prepared with procedure P_1 or P_2.

A *prepare-and-measure contextuality scenario* is an experiment consisting of performing one of X preparation procedures on a system and then one of Y measurement procedures. Mixtures of the preparation procedures assigned to each label $x \in [X]$ must satisfy some operational equivalences that are specified by the scenario. These preparation equivalences are of the form

$$\sum_x \alpha_x P_x \simeq \sum_x \beta_x P_x \tag{5}$$

for $\alpha_x \geq 0$, $\beta_x \geq 0$ such that $\sum_x \alpha_x = \sum_x \beta_x = 1$. For example, a contextuality scenario could have $X = 4$ preparations, P_j for $j \in [4]$, that must satisfy $\frac{1}{2}P_1 + \frac{1}{2}P_2 \simeq \frac{1}{2}P_3 + \frac{1}{2}P_4$. A valid realization of this experiment could be to use a qubit system with P_1 and P_2 being the eigenstates the Pauli-Z operator, while P_3 and P_4 are the eigenstates of the Pauli-X operator.

Generally, a prepare-and-measure contextuality scenario is identified by a tuple $(X, Y, B, \mathcal{OE}_P, \mathcal{OE}_M)$ indicating that it concerns X preparations satisfying equivalences $\mathcal{OE}_P$ and Y measurements each with B outcomes satisfying equivalences $\mathcal{OE}_M$. Since we only consider preparation equivalences we will omit the final element of the tuple.

We are interested in the achievable correlations within a given theory in each contextuality scenario. Each correlation is described by a vector $q \in \mathbb{R}^{XYB}$ with entries given by the probability $q(b|x,y)$ of seeing outcome b after performing measurement y on a system prepared with procedure x. We will call these vectors *behaviors* to distinguish them from the correlations in Bell scenarios.

A behavior, q, is in the set of *contextual* behaviors (i.e., behaviors realizable in some contextual theory) if for every equivalence of the form in Eq. (5) in $\mathcal{OE}_P$ the behavior satisfies

$$\sum_x \alpha_x q(b|x,y) = \sum_x \beta_x q(b|x,y) \quad \forall\, b, y. \tag{6}$$

The set of contextual behaviors contains both the sets of quantum and noncontextual behaviors (see below). A behavior, q, is in the quantum set, $\mathcal{Q}$, of a contextuality scenario $(X, Y, B, \mathcal{OE}_P)$ if

$$q(b|x,y) = \mathrm{Tr}(N_b^y \rho_x) \tag{7}$$

for some positive-operator-valued measures $N^y = \{N_b^y\}_b$ on a separable Hilbert space $\mathcal{H}$ and density operators ρ_x on $\mathcal{H}$ satisfying $\sum_x \alpha_x \rho_x = \sum_x \beta_x \rho_x$ for every equivalence of the form in Eq. (5) in $\mathcal{OE}_P$.

A subset of the quantum set (considered "classical" in contextuality scenarios) is the *noncontextual set* of behaviors. A behavior, q, is in the noncontextual set if there exists a measurable space (Λ, Σ), probability measures $\mu_x\colon \Sigma \to [0,1]$ satisfying $\sum_x \alpha_x \mu_x(E) = \sum_x \beta_x \mu_x(E)$ for every equivalence relation of the form (5) in $\mathcal{OE}_P$, and so-called *response functions* $\xi_y(b|\cdot)$ for all b and y on Λ, and $\sum_b \xi(b|E) = 1$ for all $E \in \Sigma$, such that

$$q(b|x,y) = \int_\Lambda \xi_y(b|\lambda) \mathrm{d}\mu_x(\lambda). \tag{8}$$

The map.—We now define an invertible map taking any no-signaling correlation p in a two-party Bell scenario to a behavior q from one of a family of contextuality scenarios. We will show that this map defines a bijection between (i) no-signaling Bell correlations and contextual behaviors, (ii) quantum Bell correlations and quantum behaviors, and (iii) local Bell correlations and noncontextual behaviors.

The basic premise is to imagine the Bell experiment (A, B, X, Y) as a prepare-and-measure experiment wherein if Alice inputs x and observes output a this constitutes a preparation procedure $P_{a|x}$ for Bob's system on which he will perform a measurement y and then observe an outcome b. Then, if we impose that Alice cannot signal to Bob, we know that the average preparation Bob receives when Alice inputs any x must be the same as the average preparation he receives when she inputs any other $x' \in [X]$. In other words, if the correlation observed in the Bell experiment is p then the preparations $\sum_a p_\mathrm{A}(a|x) P_{a|x}$ must be equivalent for all x, where $p_\mathrm{A}(a|x) = \sum_b p(a,b|x,y)$ for any y is the marginal distribution of Alice, which is well-defined due to no-signaling.

Thus, under the no-signaling assumption, a Bell scenario (A,B,X,Y) implements a contextuality scenario $(AX, Y, B, \mathcal{NS}(p_\mathrm{A}))$, where $\mathcal{NS}(p_\mathrm{A})$ denotes the preparation equivalences

$$\sum_a p_\mathrm{A}(a|1) P_{a|1} \simeq \cdots \simeq \sum_a p_\mathrm{A}(a|X) P_{a|X} \tag{9}$$

implied by the no-signaling assumption, which we will encode in the Cartesian product of X vectors in $\mathbb{R}^A$, where the ath element of the xth vector is $p_\mathrm{A}(a|x)$.

Based on this intuition we define our map for Bell correlations with nonzero marginal distributions for Alice. A correlation p from a Bell scenario (A,B,X,Y) is mapped to a behavior q in the contextuality scenario $(AX, Y, B, \mathcal{NS}(p_\mathrm{A}))$, where

$$q(b|[a|x], y) = \frac{p(a,b|x,y)}{p_\mathrm{A}(a|x)}. \tag{10}$$

Explicitly, our map is

$$\Gamma\colon [\mathbb{R}^{ABXY}, \mathbb{N}^4] \to \left[\mathbb{R}^{AXYB}, \mathbb{N}^3, (\mathbb{R}^A)^X\right],$$
$$[p, (A,B,X,Y)] \mapsto [q, (AX, Y, B, \mathcal{NS}(p_\mathrm{A}))], \tag{11}$$

for p in the no-signaling set of (A,B,X,Y) such that $p_\mathrm{A}(a|x) \neq 0$ where q is defined in Eq. (10).

Notice that the correlations from one Bell scenario are mapped to behaviors from multiple different contextuality scenarios. Each of the contextuality scenarios in the image of a Bell scenario (A,B,X,Y) has AX preparations and Y measurements with B outcomes but the preparation equivalences vary depending on Alice's marginal distribution in the argument correlation. This relationship is depicted in Fig. 1.

We can now define the inverse to our map. Given a contextuality scenario with preparation equivalences satisfying the following criteria, we can always express the equivalences as in Eq. (9): (i) comprising a number, X, of mixtures each of the same number, A, of preparations [since we are considering the case in which $p_\mathrm{A}(a|x) \neq 0$ for all a and x] that are all equivalent to one another, and (ii) where no preparation appears in more than one mixture.

The domain of our inverse map will be pairs of a contextuality scenario with such equivalences and a behavior in that scenario. Explicitly, the inverse of our map is then

$$\Gamma^{-1}\colon \left[\mathbb{R}^{AXYB}, \mathbb{N}^3, (\mathbb{R}^A)^X\right] \to [\mathbb{R}^{ABXY}, \mathbb{N}^4],$$
$$[q, (AX, Y, B, \mathcal{NS}(p_\mathrm{A}))] \mapsto [p, (A,B,X,Y)], \tag{12}$$

for a behavior q in the contextual set $\mathcal{C}$ of $(AX, Y, B, \mathcal{NS}(p_\mathrm{A}))$ and with $p(a,b|x,y) = p_\mathrm{A}(a|x) q(b|[a|x], y)$. Note that the $p_\mathrm{A}(a|x)$ are defined by the coefficients in the preparation equivalences of the contextuality scenario, but end up being equal to the marginals of Alice in the Bell scenario resulting in no conflict of notation.

In Sec. I of the Supplemental Material we extend the map Γ to all no-signaling correlations in a given two-party Bell scenario. In this general case, we allow zeroes in the vectors $\mathcal{NS}(p_\mathrm{A})$ leading to the same contextuality scenario appearing multiple times in the image of the map, but we use the vectors $\mathcal{NS}(p_\mathrm{A})$ to index the multiple appearances and allow the map to be invertible. Two Bell correlations that are mapped to the same behavior in two instances of a contextuality scenario are equivalent up to relabeling.

Under this extension the contextuality scenarios in the image of the map no longer are required to have the same number of preparations in each mixture in the preparation equivalences. That is, criterion (i) for a contextuality scenario to be in the domain of Γ^{-1} simply becomes a number, X, of mixtures of preparations that are all equivalent to one another.

We prove our main results about the map in the Supplemental Material. Namely, in Sec. II we prove that (given a contextuality scenario of the right type) Γ^{-1} maps every quantum contextual behavior q to a quantum spatial correlation p. We do so by observing that the problem is equivalent to finding a way to steer Bob's system into the assemblage given by the quantum states in the realization of q. The Schrödinger-HJW theorem [27] then provides an explicit construction for realizing the quantum correlation p. Section III shows that Γ maps quantum spatial correlations to quantum contextual behaviors. Then Secs. IV and V treat the cases of local and no-signaling correlations invertibly mapping to noncontextual and contextual behaviors, respectively.

Limitations of the map.—In the literature, it is claimed that any contextuality scenario with preparation equivalences given by multiple decompositions of a single hypothetical preparation

$$P_\mathrm{B} \simeq \sum_{a=1}^{Z} p_{a,1} P_a \simeq \sum_{a=1}^{Z} p_{a,2} P_a \simeq \ldots \simeq \sum_{a=1}^{Z} p_{a,X} P_a \tag{13}$$

is equivalent to a Bell scenario interpreted as a remote prepare-and-measure experiment [[5], Sec. VII]. In Sec. VI of the Supplemental Material, we give an example of a sequence of preparation equivalences of the form in Eq. (13) that cannot be reduced to a sequence of equivalences $\mathcal{NS}(p_\mathrm{A})$ [even when allowing for the coefficients $p_\mathrm{A}(a|x)$ to be zero], i.e., in our example a single preparation appears in multiple different mixtures. One can still attempt to map such a scenario, H, to a Bell scenario, by embedding behaviors q from H into those from a larger scenario H' (yielding a behavior q'), in which each appearance of a preparation that appears multiple times in $\mathcal{OE}_P$ is treated as a distinct preparation. The resulting sequence of equivalences $\mathcal{OE}'_P$ is of the form $\mathcal{NS}(p_\mathrm{A})$. However, we show via an explicit example that this embedding can map a contextual behavior q_c in H to a noncontextual behavior q'_c in H'. Thus, using this embedding to connect H to a Bell scenario leads to a contextual behavior (q_c) being mapped to a local correlation [through the embedding q'_c and then Eq. (12)]. Therefore, the connection between noncontextuality and locality would be lost by composing this embedding and our map Γ.

The quantum set in contextuality scenarios.—Using the connection we have made between the sets of quantum behaviors in contextuality scenarios and quantum correlations in Bell scenarios, we can transfer various results about quantum nonlocality to contextuality. Our main results about the quantum contextual set are given in the following four corollaries with proofs in Secs. VII–X of the Supplemental Material.

Corollary 1: The membership problem for the set of quantum behaviors in a contextuality scenario is undecidable.

Corollary 2: The set of behaviors deriving from finite-dimensional quantum systems in contextuality scenarios is a strict subset of its infinite-dimensional counterpart.

Corollary 3: In general, the set of behaviors in a contextuality scenario is not closed.

Corollary 4: No hierarchy of SDPs converges to the quantum contextual set $\mathcal{Q}$ or its closure $\overline{\mathcal{Q}}$ for all contextuality scenarios.

Note that the SDP hierarchy in Corollary 4 could be replaced by any algorithm capable of verifying that a behavior is ε away from $\mathcal{Q}$ (in ℓ_1 distance) for all $\varepsilon > 0$.

Conclusion and outlook.—We constructed an isomorphism between the set of quantum spatial correlations and the set of quantum contextual behaviors from an indexed family of contextual scenarios. This map allows us to characterize quantum nonlocality in terms of quantum contextuality, translate results from Bell nonlocality to generalized contextuality, and also raises questions about the limits of SDP hierarchies in contextuality scenarios (see the Introduction). A natural future research direction would be to investigate whether other results from Bell nonlocality, such as self-testing [28] and device-independent quantum key distribution [3], have analogs in contextuality scenarios that can be found via our construction. Lastly, one might attempt to generalize our map to multipartite Bell scenarios. One such natural generalization remains a bijection between local and noncontextual, and between no-signaling and contextual sets in multipartite Bell scenarios. However, whether this map also preserves quantumness remains unknown, with the existence of postquantum steering [29] posing an obstacle to generalizing our argument.

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Correction: A typographical error in the last sentence of the fifth paragraph has been fixed.