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Colbeck, Roger Andrew orcid.org/0000-0003-3591-0576 and Renner, Renato (2017) A system's wave function is uniquely determined by its underlying physical state. New Journal of Physics. 013016. ISSN 1367-2630

https://doi.org/10.1088/1367-2630/aa515c

A system's wave function is uniquely determined by its underlying physical state

Roger Colbeck[1,*] and Renato Renner[2,†]

[1]*Department of Mathematics, University of York, YO10 5DD, UK*

[2]*Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland*

(Dated: January 13, 2017)

We address the question of whether the quantum-mechanical wave function Ψ of a system is uniquely determined by any complete description Λ of the system's physical state. We show that this is the case if the latter satisfies a notion of "free choice". This notion requires that certain experimental parameters—those that according to quantum theory can be chosen independently of other variables—retain this property in the presence of Λ. An implication of this result is that, among all possible descriptions Λ of a system's state compatible with free choice, the wave function Ψ is as objective as Λ.

I. INTRODUCTION

The quantum-mechanical wave function, Ψ, has a clear operational meaning, specified by the Born rule [1]. It asserts that the outcome X of a measurement, defined by a family of projectors $\{\Pi_x\}$, follows a distribution P_X given by $P_X(x) = \langle\Psi|\Pi_x|\Psi\rangle$, and hence links the wave function Ψ to observations. However, the link is probabilistic: even if Ψ is known to arbitrary precision, we cannot in general predict X with certainty.

In classical physics, such indeterministic predictions are always a sign of incomplete knowledge.[1] This raises the question of whether the wave function Ψ associated to a system corresponds to an *objective* property of the system, or whether it should instead be interpreted *subjectively*, i.e., as a representation of our (incomplete) knowledge about certain underlying objective attributes. Another alternative is to deny the existence of the latter, i.e., to give up the idea of an underlying reality completely.

Despite its long history, no consensus about the interpretation of the wave function has been reached. A subjective interpretation was, for instance, supported by the famous argument of Einstein, Podolsky and Rosen [2] (see also [3]) and, more recently, by information-theoretic considerations [4–6]. The opposite (objective) point of view was taken, for instance, by Schrödinger (at least initially), von Neumann, Dirac, and Popper [7–9].

To turn this debate into a more technical question, one may consider the following gedankenexperiment: Assume you are provided with a set of variables Λ that are intended to describe the physical state of a system. Suppose, furthermore, that the set Λ is *complete*, i.e., there is nothing that can be added to Λ to increase the accuracy of any predictions about the outcomes of measurements on the system. If you were now asked to specify the wave function Ψ of the system, would your answer be unique?

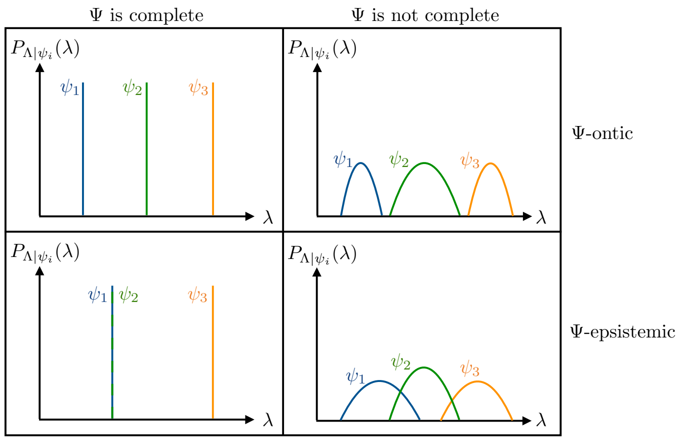

FIG. 1: *The different possible roles of the wave function Ψ.* A model that uses a variable Λ to describe a system's physical state can be either Ψ-ontic or Ψ-epistemic, depending on whether or not the wave function Ψ is uniquely determined by Λ (which takes values denoted by λ). Conversely, the relevant parts of Λ may be determined by Ψ, in which case Ψ is complete. Using free choice (with respect to an appropriate causal order), [17] rules out the right column, [16] rules out the bottom left case, and the present paper (as well as [14], based on different assumptions) rules out the bottom row.

If so then Ψ is a function of the variables Λ and hence as objective as Λ. The model defined by Λ would then be called *Ψ-ontic* [10]. Conversely, the existence of a complete set of variables Λ that does not determine the wave function Ψ would mean that Ψ cannot be interpreted as an objective property. Λ would then be called *Ψ-epistemic* (see Fig. 1).[2]

* `roger.colbeck@york.ac.uk`

† `renner@phys.ethz.ch`

[1] For example, when we assign a probability distribution P to the outcomes of a die roll, P is not an objective property but rather a representation of our incomplete knowledge. Indeed, if we had complete knowledge, including for instance the precise movement of the thrower's hand, the outcome would be deterministic.

[2] Note that the existence or non-existence of Ψ-epistemic theories is also relevant in the context of simulating quantum systems. Here Λ can be thought of as the internal state of a computer performing the simulation, and one would ideally like that storing Λ requires significantly fewer resources than would be required to store Ψ. However, a number of existing results already cast

In a seminal paper [14], Pusey, Barrett and Rudolph showed that any complete model Λ is Ψ-ontic if it satisfies an assumption, termed "preparation independence". It demands that Λ consists of separate variables for each subsystem, e.g., $\Lambda = (\Lambda_A, \Lambda_B)$ for two subsystems S_A and S_B, and that these are statistically independent, i.e., $P_{\Lambda_A \Lambda_B} = P_{\Lambda_A} P_{\Lambda_B}$, whenever the joint wave function Ψ of the total system has product form, i.e., $\Psi = \Psi_A \otimes \Psi_B$.

Here we show that the same conclusion can be reached without imposing any internal structure on Λ. In more detail, our argument relies on the concept of free choice, which can only be defined with reference to an ordering, called here a *causal order*[3]. More precisely, we prove that Ψ is a function of any complete set of variables that are compatible with free choice with respect to the causal order of Figure 3 (see later for more details). This is stated as Corollary 1. The free choice assumption used captures the idea that experimental parameters, e.g., which state to prepare or which measurement to carry out, can be chosen independently of all other information (relevant to the experiment), except for information that is created after the choice is made, e.g., measurement outcomes. While this notion is implicit in quantum theory, we demand that it also holds in the presence of Λ.[4]

The proof of our result is inspired by our earlier work [16] in which we observed that the wave function Ψ is uniquely determined by any complete set of variables Λ, provided that Ψ is itself complete (in the sense described above). Together with the result of [17], in which we showed that Ψ is complete, we can conclude that the wave function Ψ is uniquely determined by Λ.

The difference in the present work is that we can circumvent one of the aspects of quantum theory required by the argument in [17]. In particular, here we prove that Ψ is determined by Λ without requiring that any quantum measurement on a system corresponds to a unitary evolution of an extended system. Being based on weaker assumptions, the resulting no-go theorem is stronger. Furthermore, the argument that the wave function Ψ is complete is quite involved and a beneficial feature of the present work is that we circumvent it[5].

II. THE UNIQUENESS THEOREM

Our argument refers to an experimental setup where a particle emitted by a source decays into two, each of which is directed towards one of two measurement devices (see Fig. 2). The measurements that are performed depend on parameters A and B, and their respective outcomes are denoted X and Y.

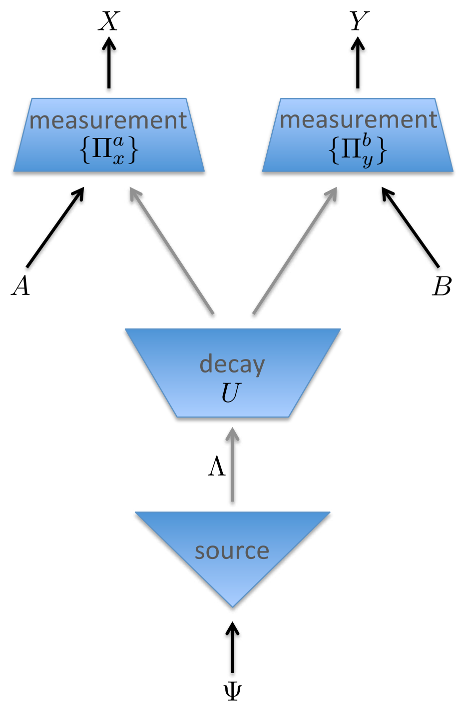

FIG. 2: *The experimental setup.* The proof of the uniqueness theorem relies on a thought experiment where a source takes as input a description of a wave function Ψ and prepares a particle in a corresponding state (which, in a general model, is described by a variable Λ). The particle then decays into two parts, which are measured at separate locations. A and B determine the measurements that are applied to the two parts, and X and Y are the respective outcomes.

Quantum theory allows us to make predictions about these outcomes based on a description of the initial state of the system, the evolution it undergoes and the measurement settings. For our purposes, we assume that the quantum state of each particle emitted by the source is pure, and hence specified by a wave function[6]. As we will consider different choices for this wave function, we model it as a random variable Ψ that takes as values unit vectors ψ in a complex Hilbert space $\mathcal{H}$. Furthermore, we take the decay to act like an isometry, denoted U, from $\mathcal{H}$ to a product space $\mathcal{H}_A \otimes \mathcal{H}_B$. Finally, for any choices a and b of the parameters A and B, the measurements are given by families of projectors $\{\Pi_x^a\}_{x \in \mathcal{X}}$ and $\{\Pi_y^b\}_{y \in \mathcal{Y}}$ on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. The Born rule, applied to this setting, now asserts that the joint probability distribution of X and Y, conditioned on the

doubt on this possibility (see, for example, [11–13]).

[3] This should not be confused with a *causal structure* as used in e.g. [15].

[4] Free choice of certain variables is also implied by the preparation independence assumption used in [14], as discussed below.

[5] Note, however, that the assumptions used in this work do not allow us to conclude that Ψ is complete.

[6] We consider it uncontroversial that a mixed state can be thought of as a state of knowledge.

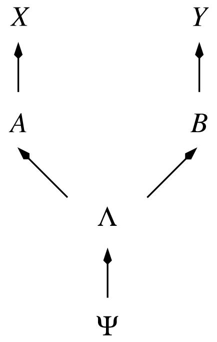

FIG. 3: *The causal order.* Free choice is only well defined if one specifies a causal order, i.e., a preorder relation on the set of variables relevant to the experiment. The causal order we use is motivated by the arrangement of variables in the experiment depicted by Fig. 2 in relativistic space time.

relevant parameters, is given by

$$P_{XY|AB\Psi}(x, y|a, b, \psi) = \langle\psi|U^\dagger(\Pi_x^a \otimes \Pi_y^b)U|\psi\rangle \ . \qquad (1)$$

To model the system's "physical state", we introduce an additional random variable Λ. We do not impose any structure on Λ (in particular, Λ could be a list of values). We will consider predictions $P_{XY|AB\Lambda}(x, y|a, b, \lambda)$ conditioned on any particular value λ of Λ, analogously to the predictions based on Ψ according to the Born rule (1).

To define the notions of *free choice* and *completeness*, as introduced informally in the introduction, we take as motivation that any experiment takes place in spacetime and therefore has a *causal order*[7]. For example, the measurement setting A is chosen before the measurement outcome X is obtained. This may be modelled mathematically by a preorder relation[8], denoted $\rightsquigarrow$, on the relevant set of random variables. While our technical claim does not depend on how the causal order is interpreted physically, it is intuitive to imagine it being compatible with relativistic spacetime. In this case, $A \rightsquigarrow X$ would mean that the spacetime point where X is accessible lies in the future light cone of the spacetime point where the choice A is made.

For our argument we consider the causal order defined by the transitive completion of the relations

$$\Psi \rightsquigarrow \Lambda, \quad \Lambda \rightsquigarrow A, \quad \Lambda \rightsquigarrow B, \quad A \rightsquigarrow X, \quad B \rightsquigarrow Y \qquad (2)$$

(cf. Fig. 3). This reflects, for instance, that Ψ is chosen at the very beginning of the experiment, and that A and B are chosen later, right before the two measurements are carried out. Note, furthermore, that $A \not\rightsquigarrow Y$ and $B \not\rightsquigarrow X$. With the aforementioned interpretation of the relation in relativistic spacetime, this would mean that the two measurements are carried out at spacelike separation.

Using the notion of a causal order, we can now specify mathematically what we mean by *free choices* and by *completeness*. We note that the two definitions below should be understood as necessary (but not necessarily sufficient) conditions characterising these concepts. Since they appear in the assumptions of our main theorem, our result also applies to any more restrictive definitions. We remark furthermore that the definitions are generic, i.e., they can be applied to any set of variables equipped with a preorder relation.[9]

Definition 1. When we say that a variable A is a *free choice from a set $\mathcal{A}$ (w.r.t. a causal order)* this means that the support of P_A contains $\mathcal{A}$ and that $P_{A|A_{\not\uparrow}} = P_A$ where $A_{\not\uparrow}$ is the set of all random variables Z (within the causal order) such that $A \not\rightsquigarrow Z$.

In other words, a choice A is free if it is uncorrelated with any other variables, except those that lie in the future of A in the causal order. For a further discussion and motivation of this notion we refer to Bell's work [19] as well as to [20].

Crucially, we note that Definition 1 is compatible with the usual understanding of free choices within quantum theory. For example, if we consider our experimental setup (cf. Fig. 2) in ordinary quantum theory (i.e., where there is no Λ), the initial state Ψ as well as the measurement settings A and B can be taken to be free choices w.r.t. $\Psi \rightsquigarrow A$, $\Psi \rightsquigarrow B$, $A \rightsquigarrow X$, $B \rightsquigarrow Y$ (which is the causal order defined by Eq. 2 with Λ removed).

Definition 2. When we say that a variable Λ is *complete (w.r.t. a causal order)* this means that[10]

$$P_{\Lambda_\uparrow|\Lambda} = P_{\Lambda_\uparrow|\Lambda\Lambda_\downarrow}$$

where $\Lambda_\uparrow$ and $\Lambda_\downarrow$ denote the sets of random variables Z (within the causal order) such that $\Lambda \rightsquigarrow Z$ and $Z \rightsquigarrow \Lambda$, respectively.

Completeness of Λ thus implies that predictions based on Λ about future values $\Lambda_\uparrow$ cannot be improved by taking into account additional information $\Lambda_\downarrow$ available in the past.[11] Recall that this is meant as a necessary criterion for completeness and that our conclusions hold for any more restrictive definition. For example, one may replace the set $\Lambda_\uparrow$ by the set of all values that are not in the past of Λ.

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[7] In previous work we sometimes called this a *chronological structure* [18].

[8] A *preorder relation* is a binary relation that is reflexive and transitive.

[9] They are therefore different from notions used commonly in the context of Bell-type experiments, such as *parameter independence* and *outcome independence*. These refer explicitly to measurement choices and outcomes, whereas no such distinction is necessary for the definitions used here.

[10] In other words, $\Lambda_\downarrow \to \Lambda \to \Lambda_\uparrow$ is a Markov chain.

[11] Using statistics terminology, one may also say that Λ is *sufficient* for $\Lambda_\uparrow$ given data $\Lambda_\downarrow$.

We are now ready to formulate our main result as a theorem. Note that, the assumptions of the theorem as well as its claim correspond to properties of the joint probability distribution of X, Y, A, B, Ψ and Λ.

Theorem 1. *Let Λ and Ψ be random variables and assume that the support of Ψ contains two wave functions, ψ and ψ', with $|\langle\psi|\psi'\rangle| < 1$. If for any isometry U and measurements $\{\Pi_x^a\}_x$ and $\{\Pi_y^b\}_y$, parameterised by $a \in \mathcal{A}$ and $b \in \mathcal{B}$, there exist random variables A, B, X and Y such that*

1. *$P_{XY|AB\Psi}$ satisfies the Born rule* (1)*;*
2. *A and B are free choices from $\mathcal{A}$ and $\mathcal{B}$, w.r.t.* (2)*;*
3. *Λ is complete w.r.t.* (2)

then there exists a subset $\mathcal{L}$ of the range of Λ such that $P_{\Lambda|\Psi}(\mathcal{L}|\psi) = 1$ and $P_{\Lambda|\Psi}(\mathcal{L}|\psi') = 0$.

The theorem asserts that, assuming validity of the Born rule and freedom of choice, the values taken by any complete variable Λ are different for different choices of the wave function Ψ. This implies that Ψ is indeed a function of Λ.

To formulate this implication as a technical statement, we consider an arbitrary countable[12] set $\mathcal{S}$ of wave functions such that $|\langle\psi|\psi'\rangle| < 1$ for any distinct elements $\psi, \psi' \in \mathcal{S}$.

Corollary 1. *Let Λ and Ψ be random variables with Ψ taking values from the set $\mathcal{S}$ of wave functions. If the conditions of Theorem 1 are satisfied then there exists a function f such that $\Psi = f(\Lambda)$ holds almost surely.*

The proof of this corollary is given in Appendix A.

III. PROOF OF THE UNIQUENESS THEOREM

The argument relies on specific wave functions, which depend on parameters $d, k \in \mathbb{N}$ and $\xi \in [0,1]$, with $k < d$. They are defined as unit vectors on a product space $\mathcal{H}_A \otimes \mathcal{H}_B$, where $\mathcal{H}_A$ and $\mathcal{H}_B$ are $(d+1)$-dimensional Hilbert spaces equipped with an orthonormal basis $\{|j\rangle\}_{j=0}^d$,[13]

$$\phi = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j\rangle|j\rangle \tag{3}$$

$$\phi' = \frac{1}{\sqrt{k}} \Big(\xi|0\rangle|0\rangle + \sum_{j=1}^{k-1} |j\rangle|j\rangle + \sqrt{1-\xi^2}|d\rangle|d\rangle \Big) . \tag{4}$$

[12] The restriction to a countable set is due to our proof technique. We leave it as an open problem to determine whether this restriction is necessary.

[13] We use here the abbreviation $|j\rangle|j\rangle$ for $|j\rangle \otimes |j\rangle$.

Lemma 1. *For any $0 \le \alpha < 1$ there exist $k, d \in \mathbb{N}$ with $k < d$ and $\xi \in [0,1]$ such that the vectors ϕ and ϕ' defined by* (3) *and* (4) *have overlap $\langle\phi|\phi'\rangle = \alpha$.*

Proof. If $\alpha = 0$, set $k = 1$, $d = 2$ and $\xi = 0$. Otherwise, set $d \ge 1/(1-\alpha^2)$, $k = \lceil \alpha^2 d \rceil$ and $\xi = \alpha\sqrt{kd} - k + 1$, so that $\xi \in [0,1]$ and $\langle\phi|\phi'\rangle = \alpha$. Furthermore, the choice of d ensures that $\alpha^2 d + 1 \le d$, which implies $k < d$. □

Furthermore, for any $n \in \mathbb{N}$, we consider projective measurements $\{\Pi_x^a\}_{x\in\mathcal{X}_d}$ and $\{\Pi_y^b\}_{y\in\mathcal{X}_d}$ on $\mathcal{H}_A$ and $\mathcal{H}_B$, parameterised by $a \in \mathcal{A}_n \equiv \{0, 2, 4, \dots, 2n-2\}$ and $b \in \mathcal{B}_n \equiv \{1, 3, 5, \dots, 2n-1\}$, and with outcomes in $\mathcal{X}_d \equiv \{0, \dots, d\}$. For $x, y \in \{0, \dots, d-1\}$, the projectors are defined in terms of the generalised Pauli operator, $\hat{X}_d \equiv \sum_{l=0}^{d-1} |l\rangle\langle l \oplus 1|$ (where $\oplus$ denotes addition modulo d) by

$$\Pi_x^a \equiv (\hat{X}_d)^{\frac{a}{2n}} |x\rangle\langle x| (\hat{X}_d^\dagger)^{\frac{a}{2n}} \tag{5}$$

$$\Pi_y^b \equiv (\hat{X}_d)^{\frac{b}{2n}} |y\rangle\langle y| (\hat{X}_d^\dagger)^{\frac{b}{2n}} \ . \tag{6}$$

We also set $\Pi_d^a = \Pi_d^b = |d\rangle\langle d|$.

The outcomes X and Y will generally be correlated. To quantify these correlations, we define[14]

$$I_{n,d}(P_{XY|AB}) \equiv 2n - \sum_{x=0}^{d-1} P_{XY|AB}(x, x\oplus 1|0, 2n-1) - \sum_{\substack{a,b \\ |a-b|=1}} \sum_{x=0}^{d-1} P_{XY|AB}(x, x|a, b).$$

For the correlations predicted by the Born rule for the measurements $\{\Pi_x^a\}_{x\in\mathcal{X}_d}$ and $\{\Pi_y^b\}_{y\in\mathcal{X}_d}$ applied to the state ϕ defined by (3), i.e., $P_{XY|AB}(x,y|a,b) = \langle\phi|\Pi_x^a \otimes \Pi_y^b|\phi\rangle$, we find (see Appendix B)

$$I_{n,d}(P_{XY|AB}) \le \frac{\pi^2}{6n} \ . \tag{7}$$

The next lemma shows that $I_{n,d}$ gives an upper bound on the distance of the distribution $P_{X|A\Lambda}$ from a uniform distribution over $\{0, \dots, d-1\}$. The bound holds for any random variable Λ, provided the joint distribution $P_{XY\Lambda|AB}$ satisfies certain conditions.

Lemma 2. *Let $P_{XYAB\Lambda}$ be a distribution that satisfies $P_{X\Lambda|AB} = P_{X\Lambda|A}$, $P_{Y\Lambda|AB} = P_{Y\Lambda|B}$ and $P_{AB\Lambda} = P_A P_B P_\Lambda$ with $\mathrm{supp}(P_A) \supseteq \mathcal{A}_n$ and $\mathrm{supp}(P_B) \supseteq \mathcal{B}_n$. Then*

$$\int \mathrm{d}P_\Lambda(\lambda) \sum_{x=0}^{d-1} \big| P_{X|A\Lambda}(x|0,\lambda) - \frac{1}{d} \big| \le \frac{d}{2} I_{n,d}(P_{XY|AB}) \, .$$

[14] Note that the first sum corresponds to the probability that $X \oplus 1 = Y$, conditioned on $A = 0$ and $B = 2n-1$. The terms in the second sum can be interpreted analogously.

(Although our proof deals with the general case, the main ideas can be seen by working through the analogous argument in the slightly simpler (but less general) case in which Λ is discrete, so that "$\int \mathrm{d}P_\Lambda(\lambda)$" is replaced by "$\sum_\lambda P_\Lambda(\lambda)$".)

The proof of Lemma 2 is given in Appendix C. It generalises an argument described in [17], which is in turn based on work related to chained Bell inequalities [21, 22] (see also [23, 24]).

We have now everything ready to prove the uniqueness theorem.

Proof of Theorem 1. Let $\alpha, \gamma \in \mathbb{R}$ such that $e^{i\gamma}\alpha = \langle\psi|\psi'\rangle$. Furthermore, let k, d, ξ be as defined by Lemma 1, so that $\langle\phi|\phi'\rangle = \alpha$. Then there exists an isometry U such that $U\psi = \phi$ and $U\psi' = e^{i\gamma}\phi'$ (see Lemma 3 of Appendix D).[15] Now let $n \in \mathbb{N}$ and let A, B, X and Y be random variables that satisfy the three conditions of the theorem for the isometry U and for the projective measurements defined by (5) and (6), which are parameterised by $a \in \mathcal{A}_n$ and $b \in \mathcal{B}_n$, respectively. According to the Born rule (Condition 1), the distribution $P_{XY|AB\psi} \equiv P_{XY|AB\Psi}(\cdot,\cdot|\cdot,\cdot,\psi)$ conditioned on the choice of initial state $\Psi = \psi$ corresponds to the one considered in (7), i.e.,

$$I_{n,d}(P_{XY|AB\psi}) \leq \frac{\pi^2}{6n} \, . \tag{8}$$

Note that $P_{A|B\Psi}P_{Y\Lambda|AB\Psi} = P_{AY\Lambda|B\Psi} = P_{A|BY\Lambda\Psi}P_{Y\Lambda|B\Psi}$. Freedom of choice (Condition 2) implies that $P_{A|B\Psi} = P_{A|BY\Lambda\Psi}$. It follows that $P_{Y\Lambda|AB\Psi} = P_{Y\Lambda|B\Psi}$. By a similar reasoning, we also have $P_{X\Lambda|AB\Psi} = P_{X\Lambda|A\Psi}$. The freedom of choice condition also ensures that $P_{AB\Lambda|\Psi} = P_A P_B P_{\Lambda|\Psi}$ with $\mathrm{supp}(P_A) \supseteq \mathcal{A}_n$ and $\mathrm{supp}(P_B) \supseteq \mathcal{B}_n$. We can thus apply Lemma 2 to give, with (8),

$$\int \mathrm{d}P_{\Lambda|\psi}(\lambda) \sum_{x=0}^{d-1} \left| P_{X|A\Lambda\Psi}(x|0,\lambda,\psi) - \frac{1}{d} \right| \leq \frac{d\pi^2}{12n} \, .$$

Considering only the term $x = k$ (recall that $k < d$) and noting that the left hand side does not depend on n, we have

$$\int \mathrm{d}P_{\Lambda|\psi}(\lambda) \left| P_{X|A\Lambda\Psi}(k|0,\lambda,\psi) - \frac{1}{d} \right| = 0$$

(otherwise, by taking n sufficiently large, we will get a contradiction with the above). Let $\mathcal{L}$ be the set of all elements λ from the range of Λ for which $P_{X|A\Lambda\Psi}(k|0,\lambda,\psi)$ is defined and equal to $\frac{1}{d}$. The above implies that $P_{\Lambda|\Psi}(\mathcal{L}|\psi) = 1$. Furthermore, completeness of Λ (Condition 3) implies that for any $\lambda \in \mathcal{L}$ for which $P_{X|A\Lambda\Psi}(k|0,\lambda,\psi')$ is defined

$$P_{X|A\Lambda\Psi}(k|0,\lambda,\psi') = P_{X|A\Lambda\Psi}(k|0,\lambda,\psi) = \frac{1}{d} \, .$$

Thus, using $P_{\Lambda|A\Psi} = P_{\Lambda|\Psi}$ (which is implied by the freedom of choice assumption, Condition 2) and writing $\delta_{\mathcal{L}}$ for the indicator function, we have

$$\begin{aligned} P_{X|A\Psi}(k|0,\psi') &= \int \mathrm{d}P_{\Lambda|\Psi}(\lambda|\psi') P_{X|A\Lambda\Psi}(k|0,\lambda,\psi') \\ &\geq \int \delta_{\mathcal{L}}(\lambda) \mathrm{d}P_{\Lambda|\Psi}(\lambda|\psi') P_{X|A\Lambda\Psi}(k|0,\lambda,\psi') \\ &= \frac{1}{d} \int \delta_{\mathcal{L}}(\lambda) \mathrm{d}P_{\Lambda|\Psi}(\lambda|\psi') = \frac{1}{d} P_{\Lambda|\Psi}(\mathcal{L}|\psi') \, . \end{aligned} \tag{9}$$

However, because the vector $e^{i\gamma}\phi' = U\psi'$ has no overlap with $|k\rangle$ (because $k < d$) and because the measurement $\{\Pi_x^a\}_{x \in \mathcal{X}_d}$ for $a = 0$ corresponds to projectors along the $\{|x\rangle\}_{x=0}^d$ basis, we have $P_{X|A\Psi}(k|0,\psi') = 0$ by the Born rule (Condition 1). Inserting this in (9) we conclude that $P_{\Lambda|\Psi}(\mathcal{L}|\psi') = 0$. $\square$

IV. DISCUSSION

It is interesting to compare Theorem 1 to the result of [14], which we briefly described in the introduction. The latter is based on a different experimental setup, where n particles with wave functions $\Psi_1, \ldots, \Psi_n$, each chosen from a set $\{\psi, \psi'\}$, are prepared independently at n remote locations. The n particles are then directed to a device where they undergo a joint measurement with outcome Z.

The main result of [14] is that, for any variable Λ that satisfies certain assumptions, the wave functions $\Psi_1, \ldots, \Psi_n$ are determined by Λ. One of these assumptions is that Λ consists of n parts, $\Lambda_1, \ldots, \Lambda_n$, one for each particle. To state the other assumptions and compare them to ours, it is useful to consider the causal order defined by the transitive completion of the relations[16]

$$\Psi_i \rightsquigarrow \Lambda_i \;\; (\forall\, i), \quad (\Lambda_1, \ldots, \Lambda_n) \rightsquigarrow \Lambda, \quad \Lambda \rightsquigarrow Z \, . \tag{10}$$

It is then easily verified that the assumptions of [14] imply the following:

1. $P_{Z|\Psi_1 \cdots \Psi_n}$ satisfies the Born rule;
2. $\Psi_1, \ldots, \Psi_n$ are free choices from $\{\psi, \psi'\}$ w.r.t. (10);
3. Λ is complete w.r.t. (10).

[15] If $\mathcal{H}$ has a larger dimension than $\mathcal{H}_A \otimes \mathcal{H}_B$ (e.g., because $\mathcal{H}$ is infinite dimensional) then we can consider an (infinite dimensional) extension of $\mathcal{H}_B$, keeping the same notation for convenience.

[16] Note that this causal order captures the aforementioned experimental setup. In particular, we have $\Psi_i \not\rightsquigarrow \Lambda_j$ for $i \neq j$, reflecting the idea that the n particles are prepared in separate isolated devices.

These conditions are essentially in one-to-one correspondence with the assumptions of Theorem 1.[17] The main difference thus concerns the modelling of the physical state Λ, which in the approach of [14] is assumed to have an internal structure. A main goal of the present work was to avoid using this assumption (see also [25, 26] for alternative arguments).

We conclude by noting that the assumptions of Theorem 1 and Corollary 1 may be weakened. For example, the independence condition that is implied by free choice may be replaced by a partial independence condition along the lines considered in [27]. An analogous weakening was given in [28, 29] regarding the argument of [14]. More generally, recall that all our assumptions are properties of the probability distribution $P_{XYAB\Psi\Lambda}$. One may therefore replace them by relaxed properties that need only be satisfied for distributions that are ε-close (in total variation distance) to $P_{XYAB\Psi\Lambda}$. (For example, the Born rule may only hold approximately.) It is relatively straightforward to verify that the proof still goes through, leading to the claim that $\Psi = f(\Lambda)$ holds with probability at least $1-\delta$, with $\delta \to 0$ in the limit where $\varepsilon \to 0$.

Nevertheless, none of the three assumptions of Theorem 1 can be dropped without replacement. Indeed, without the Born rule, the wave function Ψ has no meaning and could be taken to be independent of the measurement outcomes X. Furthermore, a recent impossibility result [30] implies that the analogous theorem with the second assumption omitted does not hold. It also implies that the statement of Theorem 1 cannot hold for a setting with only one single measurement. This means that there exist Ψ-epistemic theories compatible with the remaining assumptions. However, in this case, it is still possible to exclude a certain subclass of such theories, called *maximally Ψ-epistemic* theories [31] (see also [32]). Finally, completeness of Λ is necessary because, without it, Λ could be set to a constant, in which case it clearly cannot determine Ψ.

Acknowledgments

We thank Omar Fawzi, Michael Hush, Matt Leifer, Matthew Pusey and Rob Spekkens for useful discussions. Research leading to these results was supported by the Swiss National Science Foundation (through the National Centre of Competence in Research *Quantum Science and Technology* and grant No. 200020-135048), the CHIST-ERA project DIQIP, and the European Research Council (grant No. 258932).

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Appendix A: Proof of Corollary 1

For any distinct $\psi, \psi' \in \mathcal{S}$, let $\mathcal{L}_{\psi,\psi'}$ be the set defined by Theorem 1, i.e.,

$$P_{\Lambda|\Psi}(\mathcal{L}_{\psi,\psi'}|\psi) = 1$$
$$P_{\Lambda|\Psi}(\mathcal{L}_{\psi,\psi'}|\psi') = 0 \ ,$$

and for any $\psi \in \mathcal{S}$ define the (countable) intersection $\mathcal{L}_\psi \equiv \bigcap_{\psi' \in \mathcal{S}\setminus\{\psi\}} \mathcal{L}_{\psi,\psi'}$. This satisfies

$$P_{\Lambda|\Psi}(\mathcal{L}_\psi|\psi') = \begin{cases} 1 & \text{if } \psi = \psi' \\ 0 & \text{otherwise.} \end{cases}$$

(Here we have used that for any probability distribution P and for any events L, L', $P(L) = P(L') = 1$ implies that $P(L \cap L') = 1$.)

To define the function f, we specify the inverse sets

$$f^{-1}(\psi) = \mathcal{L}_\psi \setminus \Big(\bigcup_{\psi' \in \mathcal{S}\setminus\{\psi\}} \mathcal{L}_{\psi'} \Big) \ .$$

The function f is well defined on $\bigcup_{\psi \in \mathcal{S}} f^{-1}(\psi)$ because, by construction, the sets $f^{-1}(\psi)$ are disjoint for different $\psi \in \mathcal{S}$. Furthermore, it follows from the above that for any $\psi \in \mathcal{S}$

$$P_{\Lambda|\Psi}(f^{-1}(\psi)|\psi) = 1 \ .$$

This implies that $f(\Lambda) = \Psi$ holds with probability 1 conditioned on $\Psi = \psi$. The assertion of the corollary then follows because this is true for any $\psi \in \mathcal{S}$. □

Appendix B: Quantum correlations

The aim of this appendix is to derive the bound (7) used in the proof of the uniqueness theorem.

Note that the state ϕ, defined by (3), has support on $\bar{\mathcal{H}} \otimes \bar{\mathcal{H}}$, where $\bar{\mathcal{H}} = \mathrm{span}\{|0\rangle, |1\rangle, \ldots, |d-1\rangle\}$. Since the projectors Π_x^a and Π_y^b, defined by (5) and (6), for $a \in \mathcal{A}_n$ and $b \in \mathcal{B}_n$ and for $x, y \in \{0, \ldots, d-1\}$ also act on $\bar{\mathcal{H}}$, we can restrict to this subspace.

For $j \in \{0, \ldots, d-1\}$ and $k \in \{0, \ldots, 2n-1\}$ the projectors Π_j^k are along the vectors

$$|\zeta_j^k\rangle = (\hat{X}_d)^{\frac{k}{2n}} |j\rangle \ ,$$

where $\hat{X}_d$ denotes the generalised Pauli operator (defined in the main text). To write these vectors out more explicitly, we consider the diagonal operator $\hat{Z}_d \equiv \sum_{j=0}^{d-1} e^{2\pi i j/d} |j\rangle\langle j|$ and the unitary $U_d \equiv \frac{1}{\sqrt{d}} \sum_{jk} e^{2\pi i jk/d} |j\rangle\langle k|$. These have the property that $\hat{X}_d = U_d \hat{Z}_d U_d^\dagger$, and hence it follows that $(\hat{X}_d)^{\frac{k}{2n}} = U_d (\hat{Z}_d)^{\frac{k}{2n}} U_d^\dagger$. Thus, we can write

$$|\zeta_j^k\rangle = \frac{1}{d} \sum_{m=0}^{d-1} \frac{1 - \exp[\frac{ik\pi}{n}]}{1 - \exp[\frac{2\pi i}{d}(m + k/2n - j)]} |m\rangle \ ,$$

for $k \neq 0$. Note that $\langle \zeta_j^k | \zeta_{j'}^k \rangle = \delta_{j,j'}$, implying that, for each k, $\{\Pi_j^k\}_j$ is a projective measurement on $\bar{\mathcal{H}}$.

Recall that the probability distribution in (7) is obtained from a measurement of ϕ with respect to these projectors, i.e., $P_{XY|AB}(x, y|a, b) = |(\langle \zeta_x^a | \langle \zeta_y^b |) |\phi\rangle|^2$. We are now going to show that

$$\sum_x P_{XY|AB}(x, x|a, b) = \frac{\sin^2 \frac{\pi}{2n}}{d^2 \sin^2 \frac{\pi}{2dn}} \ , \tag{B1}$$

for $|a - b| = 1$, and

$$\sum_x P_{XY|AB}(x, x \oplus 1|0, 2n-1) = \frac{\sin^2 \frac{\pi}{2n}}{d^2 \sin^2 \frac{\pi}{2dn}} \ . \tag{B2}$$

For this it is useful to use the relation that for any operator C, $(\mathbb{1} \otimes C)|\phi\rangle = (C^{\mathrm{T}} \otimes \mathbb{1})|\phi\rangle$, where C^{T} denotes the transpose of C in the $|i\rangle$ basis. Thus, noting that $U_d^{\mathrm{T}} = U_d$, we have

$$(\langle \zeta_x^a | \langle \zeta_x^b |) |\phi\rangle = \frac{1}{\sqrt{d}} \langle x | U_d \hat{Z}_d^{\frac{a}{2n}} (U_d^\dagger)^2 \hat{Z}_d^{\frac{b}{2n}} U_d | x \rangle \ .$$

Then, using

$$(U_d^\dagger)^2 = \frac{1}{d} \sum_{jkm} e^{-2\pi i j(k+m)/d} |k\rangle\langle m| = \sum_{k=0}^{d-1} |k\rangle\langle -k \oplus d| \ ,$$

we find

$$|(\langle \zeta_x^a | \langle \zeta_x^b |) |\phi\rangle| = \frac{1}{d^{3/2}} \sum_j e^{\frac{\pi i j}{dn}(a-b)} = \frac{1}{d^{3/2}} \frac{1 - e^{\frac{\pi i}{n}(a-b)}}{1 - e^{\frac{\pi i}{dn}(a-b)}} \ .$$

We can hence use $|1 - e^{iy}|^2 = 4 \sin^2 \frac{y}{2}$ to obtain

$$\sum_x P_{XY|AB}^{n,d}(x, x|a, b) = \frac{\sin^2 \frac{\pi(a-b)}{2n}}{d^2 \sin^2 \frac{\pi(a-b)}{2dn}} \ ,$$

from which (B1) follows. (B2) can be obtained by a similar argument. These two expressions immediately imply

$$I_{n,d}(P_{XY|AB}) = 2n(1 - \frac{\sin^2 \frac{\pi}{2n}}{d^2 \sin^2 \frac{\pi}{2dn}}) \, .$$

Using $x^2 - x^4/3 \leq \sin^2 x \leq x^2$ for $0 \leq x \leq 1$ leads to the bound (7).

Appendix C: Proof of Lemma 2

In the following we use the abbreviations $P_{XY|AB\lambda} \equiv P_{XY|AB\Lambda}(\cdot,\cdot|\cdot,\cdot,\lambda)$ and $P_{XY|ab\lambda} = P_{XY|AB\lambda}(\cdot,\cdot|a,b)$ for the distributions conditioned on $\Lambda = \lambda$ and $(A,B) = (a,b)$.

The inequality in Lemma 2 can be expressed in terms of the total variation distance, defined by $D(P_X, Q_X) \equiv \frac{1}{2}\sum_x |P_X(x) - Q_X(x)|$, as

$$\int \mathrm{d}P_\Lambda(\lambda) D(P_{X|a_0\lambda}, 1/d) \leq \frac{d}{4} I_{n,d}(P_{XY|AB}) \, .$$

where $1/d$ denotes the uniform distribution over $\{0,\ldots,d-1\}$, and where $a_0 = 0$. Furthermore, using $P_{XY|AB} = \int \mathrm{d}P_\Lambda(\lambda) P_{XY|AB\lambda}$ (which holds because $P_{\Lambda|AB} = P_\Lambda$) and that $I_{n,d}$ is a linear function, we have

$$I_{n,d}(P_{XY|AB}) = \int \mathrm{d}P_\Lambda(\lambda) I_{n,d}(P_{XY|AB\lambda}) \, .$$

It therefore suffices to show that, for any λ,

$$D(P_{X|a_0\lambda}, 1/d) \leq \frac{d}{4} I_{n,d}(P_{XY|AB\lambda}) \, .$$

For this, we consider the distribution $P_{X\oplus 1|a\lambda}$, which corresponds to the distribution of X if its values are shifted by one (modulo d). According to Lemma 5 and using $\frac{1}{d}\lfloor\frac{d^2}{4}\rfloor \leq \frac{d}{4}$ we have

$$D(P_{X|a_0\lambda}, 1/d) \leq \frac{d}{4} D(P_{X\oplus 1|a_0\lambda}, P_{X|a_0\lambda}) \, .$$

The assertion then follows with

$$\begin{aligned}
& I_{n,d}(P_{XY|AB\lambda}) \\
& = 2n - \sum_x P_{XY|a_0 b_0 \lambda}(x, x\oplus 1) - \sum_{\substack{x,a,b \\ |a-b|=1}} P_{XY|ab\lambda}(x,x) \\
& \geq D(P_{X\oplus 1|a_0 b_0\lambda}, P_{Y|a_0 b_0 \lambda}) + \sum_{\substack{a,b \\ |a-b|=1}} D(P_{X|ab\lambda}, P_{Y|ab\lambda}) \\
& \geq D(P_{X\oplus 1|a_0\lambda}, P_{X|a_0\lambda}) \, ,
\end{aligned}$$

where we have set $b_0 \equiv 2n-1$; the first inequality follows from Lemma 4; the second is obtained with $P_{X|ab\lambda} = P_{X|a\lambda}$ and $P_{Y|ab\lambda} = P_{Y|b\lambda}$ (which are implied by the conditions stated in the lemma) as well as the triangle inequality for $D(\cdot,\cdot)$. □

Appendix D: Additional Lemmas

Lemma 3. *For any unit vectors $\psi, \psi' \in \mathcal{H}_1$ and $\phi, \phi' \in \mathcal{H}_2$, where $\dim(\mathcal{H}_1) \leq \dim(\mathcal{H}_2)$ and $\langle\psi|\psi'\rangle = \langle\phi|\phi'\rangle$, there exists an isometry $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $U\psi = \phi$ and $U\psi' = \phi'$.*

Proof. With $\alpha = \langle\psi|\psi'\rangle = \langle\phi|\phi'\rangle$ and $\beta = \sqrt{1-|\alpha|^2}$ we can write $\psi' = \alpha\psi + \beta\psi^\perp$ and $\phi' = \alpha\phi + \beta\phi^\perp$ with unit vectors $\psi^\perp$ and $\phi^\perp$ orthogonal to ψ and ϕ, respectively. The isometry U can be taken as any that acts as $|\phi\rangle\langle\psi| + |\phi^\perp\rangle\langle\psi^\perp|$ on the subspace spanned by ψ and ψ'. □

Lemma 4. *For two random variables X and Y with joint distribution P_{XY}, the total variation distance between the marginal distributions P_X and P_Y satisfies*

$$D(P_X, P_Y) \leq 1 - \sum_x P_{XY}(x,x) \, .$$

Proof. Consider $P^{\neq}_{XY} \equiv P_{XY|X\neq Y}$, the distribution of X and Y conditioned on the event that $X \neq Y$, as well as $P^{=}_{XY} \equiv P_{XY|X=Y}$ so that

$$P_{XY} = p_{\neq} P^{\neq}_{XY} + (1-p_{\neq}) P^{=}_{XY}$$

where $p_{\neq} \equiv 1 - \sum_x P_{XY}(x,x)$. The marginals also obey this relation, i.e.,

$$\begin{aligned}
P_X &= p_{\neq} P^{\neq}_X + (1-p_{\neq}) P^{=}_X \\
P_Y &= p_{\neq} P^{\neq}_Y + (1-p_{\neq}) P^{=}_Y \, .
\end{aligned}$$

Hence, since the total variation distance is convex,

$$\begin{aligned}
D(P_X, P_Y) &\leq p_{\neq} D(P^{\neq}_X, P^{\neq}_Y) + (1-p_{\neq}) D(P^{=}_X, P^{=}_Y) \\
&\leq p_{\neq} \, ,
\end{aligned}$$

where we have used the fact that the total variation distance is at most 1, as well as $D(P^{=}_X, P^{=}_Y) = 0$ in the last line. □

Lemma 5. *The total variation distance between any probability distribution with range $\{0, 1, \ldots, d-1\}$ and the uniform distribution over this set, $1/d$, is bounded by*

$$D(P_X, 1/d) \leq \frac{1}{d}\lfloor\frac{d^2}{4}\rfloor D(P_{X\oplus 1}, P_X) \, .$$

Proof. Using $\frac{1}{d}\sum_{i=0}^{d-1} P_{X\oplus i} = 1/d$ and the convexity of D, we find

$$\begin{aligned}
D(P_X, 1/d) &= D(\frac{1}{d}\sum_{i=0}^{d-1} P_X, \frac{1}{d}\sum_{i=0}^{d-1} P_{X\oplus i}) \\
&\leq \frac{1}{d}\sum_{i=0}^{d-1} D(P_X, P_{X\oplus i}) \, .
\end{aligned}$$

Because $D(P_{X\oplus(i-1)}, P_{X\oplus i}) = D(P_{X\oplus 1}, P_X)$ for all i we have for $i \leq d/2$

$$\begin{aligned} D(P_X, P_{X\oplus i}) &\leq D(P_X, P_{X\oplus(i-1)}) + D(P_{X\oplus(i-1)}, P_{X\oplus i}) \\ &= D(P_X, P_{X\oplus(i-1)}) + D(P_{X\oplus 1}, P_X) \ . \end{aligned}$$

Using this multiple times yields $D(P_X, P_{X\oplus i}) \leq iD(P_{X\oplus 1}, P_X)$. Similarly, for $i \geq d/2$, we use

$$\begin{aligned} D(P_X, P_{X\oplus i}) &\leq D(P_X, P_{X\oplus(i+1)}) + D(P_{X\oplus(i+1)}, P_{X\oplus i}) \\ &= D(P_X, P_{X\oplus(i+1)}) + D(P_{X\oplus 1}, P_X) \end{aligned}$$

multiple times to yield $D(P_X, P_{X\oplus i}) \leq (d-i)D(P_{X\oplus 1}, P_X)$. Thus,

$$\begin{aligned} &\sum_{i=0}^{d-1} D(P_X, P_{X\oplus i}) \\ &\quad \leq \left(\sum_{i=0}^{\lfloor d/2 \rfloor} i + \sum_{i=\lfloor d/2 \rfloor+1}^{d-1} (d-i) \right) D(P_{X\oplus 1}, P_X) \\ &\quad = \left\lfloor \frac{d^2}{4} \right\rfloor D(P_{X\oplus 1}, P_X) \, . \end{aligned}$$

Combining this with the above concludes the proof. □

Note that there are distributions that achieve the bound of Lemma 5, as can be seen for d even and the distribution $P_X = (2/d, 2/d, \ldots, 2/d, 0, 0, \ldots)$, for which $D(P_X, 1/d) = 1/2$ and $D(P_{X\oplus 1}, P_X) = 2/d$.