Quantum Foundations: No-Go Theorems of ψ-Ontological Quantum Models

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Abstract

This paper delves into the foundations of quantum mechanics, the limitations of ontological models in explaining quantum phenomena. We first define what it means for a model of quantum mechanics to be "real". This is mathematically defined as "ψ-ontology". The report discusses Bell's inequality, measurement contextuality using the Kochen-Specker theorem, and the Pusey-Barrett-Rudolph (PBR) theorem is also explored. Notable, the PBR theorem rejects a certain class of ψ-ontological models of quantum mechanics. The paper provides a comprehensive overview of the mathematical formalism that underpin these no-go theorems, highlighting the fundamental strangeness of quantum mechanics.

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1 Introduction

The discovery of quantum mechanics was a profound shock to the scientific community. In 1927, German physicist Werner Heisenberg demonstrated that classical physics did not apply at the atomic level (Beyler). Heisenberg showed that a particle's location and velocity were varying quantities: similarly prepared particles will fundamentally obey some statistical distribution of position and momentum upon measurement, rather than some fixed position and momentum as dictated by classical mechanics. This infamous rule is termed the Heisenberg uncertainty principle. Heisenberg's discovery and many other experimental results revolutionised the way physicists thought about the natural world.

Quantum mechanics is founded on a set of fundamental postulates that describe the behaviour of microscopic particles (see Appendix 8.1). What sets quantum mechanics apart from classical physics is its intriguing approach to the observer and the observed. Unlike classical physics, which views the observer as an objective and passive entity, separate from the observed reality, quantum mechanics recognizes the active role that the act of observation plays in shaping the observed reality, making it a crucial postulate of the theory.

Despite a century of research, however, there is no consensus on how to interpret the postulates of quantum mechanics. What is the mechanism by which the postulates work? Some physicists believe that the quantum physics represents an objective description of reality mirroring classical physics, while others believe that it is merely a mathematical tool for making predictions. This ongoing debate highlights the deeply philosophical conundrum that quantum mechanics poses.

Experimentally, there did not seem to be a way to explain the postulates of quantum mechanics. The postulates seem to be basic experimental facts about the world. Some are not satisfied with this explanation, however, and developed frameworks to explain the mechanisms behind the postulates of quantum mechanics. Such frameworks are termed the interpretations of quantum mechanics. All consistent interpretations are experimentally the same; they reproduce the results of quantum mechanics. However, interpretations are conceptually and theoretically distinct.

In this paper, we will be examining a subgroup of such interpretations of quantum mechanics, termed the "ψ-ontological models", through the lens of quantum foundations. The field of quantum foundations is interested in categorising interpretations of quantum mechanics in a mathematical framework and developing mathematical theories which tells us the implications of theories within this framework. We will explore the various no-go theorems that mathematically restrict the properties of such "ψ-ontological models". We will also cover the Pusey-Barrett-Rudolph (PBR) theorem, a new result published in 2012 which some have termed "the most important general theorem relating to the foundations of quantum mechanics since Bell's theorem" (Reich).

2 Bell's Inequality

The advent of quantum mechanics challenged the notion in classical physics that physical properties exists independently of observation. In classical physics, a particle's physical state is uniquely specified by its position and momentum, which have definite values. Ideally, we can measure these properties to identify the physical state of the particle. In contrast, measurement becomes a fundamental concept in quantum mechanics, influencing the way we interact with and gain information about the world, rather than just being a means of probing the underlying reality. The notion of a physical state is dubious within the context of quantum mechanics, as it does not make sense to discuss the state of a quantum system prior to measurement. However, some disagreed with the notion that there was no underlying reality. In a famous paper by Albert Einstein, Nathan Rosen, and Boris Podolsky (EPR, based on their surnames), the EPR paper proposed a thought experiment that aimed to demonstrate that quantum mechanics is not a complete theory of nature (Nielsen and Chuang 112).

As the EPR paper implied, given an entangled pair of qubits in the Bell basis:

$$\frac{|01\rangle - |10\rangle}{\sqrt{2}}, \tag{1}$$

if we give Alice the first qubit and Bob had the second qubit, if Alice applies some any possible measurement and measures the eigenvalue $+1$, then she can easily predict that Bob will measure -1 if he does the same measurement (see Appendix 8.3).

The EPR paper put forward a criterion according to which a physical property must be considered an "element of reality" if Alice can always predict the outcome of a measurement on Bob's qubit. The aim of the EPR argument was to demonstrate the incompleteness of quantum mechanics by pointing out the absence of such an "element of reality" (114). This was meant to prompt a reconsideration of the classical worldview, which posited the feasibility of attributing properties to systems independent of measurements. However, this criterion was challenged by a mathematical discovery that emerged approximately three decades later, providing support for the principles of quantum mechanics over classical physics (114).

The following theorem, known as Bell's inequality, is a mathematical deduction based on a set of assumptions about reality. By reaching a contradiction, we show that our assumptions are inconsistent. We outline Nielsen and Chuang's proof of Bell's theorem (114).

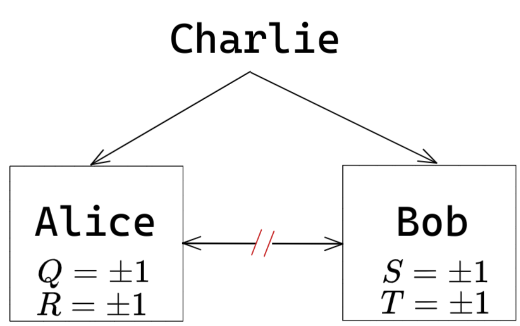

Figure 1: The experimental demonstration of Bell's inequalities involves a schematic setup where Alice and Bob are assumed to be sufficiently far apart that the measurement of one system cannot affect the other's outcome. In this setup, Alice chooses to measure either Q or R, while Bob chooses to measure either S or T. These measurements are performed simultaneously, and the outcomes are recorded. Adapted from Nielsen and Chuang (114).

The experiment (depicted in Figure 1) involves Charlie preparing two particles, which he then sends to Alice and Bob. Alice performs a measurement on her particle, selecting either of two possible measurements we label P_Q and P_R, which respectively correspond to physical properties (we assume) which are observer independent. The outcomes of these measurements are either

+1 or −1. Alice does not know in advance which measurement she will perform, and selects it randomly upon receiving the particle. The value Q is a physical property of Alice's particle, and similarly, R represents the value revealed by a measurement of the property P_R (114).

Bob is capable of measuring one of two properties, P_S or P_T , which reveals an objectively existing value S or T for the property, each taking value +1 or −1. Bob selects the measurement randomly upon receiving the particle. Alice and Bob perform their measurements at the same time, in a causally disconnected manner, such that one measurement cannot disturb the other. This is done by placing them far away, since we know that any physical influences cannot propagate faster than light, per the principles of relativity (115).

According to Nielsen and Chuang (115), we can construct expectation values on the physical properties (see Appendix 8.4). In our construction, we make two definite assumptions. The first is that Q, R, S, T are physical properties with definite values. The second is that Alice's measurement does not affect Bob's measurement. The second assumption is the principle of locality (117). In quantum mechanics, the bounds of the expectation based on the above two assumptions are violated for the possible properties of the system we measure. For example, the measurable property of a qubit is its state-vector in some measurement basis. From Appendix 8.4, we see that there exists choices of Q, R, S, T which violate the bound we set on the expectation value, which suggests that the measurable properties are not physical.

For this theorem, we have assumed that our theory of quantum mechanics must contain physical properties. The violation of Bell's inequality suggests that theories of quantum mechanics which assumes physical properties of systems must be non-local. Thus, local realism is theoretically and experimentally not possible. More exactly, we cannot develop a local "hidden variable theory" whose results reproduce quantum mechanics. This is a very important restriction on such realist models of quantum mechanics.

The violation of Bell's inequality by quantum mechanics has strong implications for the types of "hidden variable theory" we can create. One may ask if other such restrictions exists for such realist models of physics? In the subsequent sections, we will understand the standard language for describing realist models of physics in the quantum foundation literature, and explore no-go theorems which enact restrictions upon such realist models.

3 ψ-Ontological Models of Quantum Mechanics

Ontology, derived from the Greek word for "being," is the branch of metaphysics concerned with the nature of things that exist (Leifer 69). In physics, an ontic state exists objectively in the world, independent of any observer or agent, whereas an epistemic state is a description of an observer's knowledge of a physical system, existing solely in the observer's mind. The epistemic state is thus some knowledge about the ontic state (69). Thus, there is a clear-cut distinction between ontic and epistemic states in classical mechanics. As described by Leifer (69), a single particle in one dimension has an objective position x and momentum p, both independent of observers. These properties, along with all other objective properties of the particle, are functions of x and p, making the ontic state of the particle the phase space point (x, p). However, if we lack knowledge of the exact position and momentum of the particle, our understanding of its ontic state is represented by a probability density $f(x, p)$ over phase space. In this scenario, $f(x, p)$ serves as our epistemic state; it gives us probabilistic knowledge about the underlying ontic state (70). Regardless of the type and dimension of the classical system, the ontic state is the phase space point, while the epistemic state is a probability density over phase space.

In quantum mechanics, we consider the following question: does the quantum state $|\psi\rangle$ corresponds to an independently existing property of the individual system or is simply a mathematical tool for calculating probabilities? This issue is highly debated in quantum foundations and is referred to as the ψ-ontic/ψ-epistemic distinction (71). The terms ψ-ontic/ψ-epistemic are used to describe interpretations that distinguish whether our quantum states corresponds to some unique part of reality, or whether it simply represents our knowledge of the underlying reality. In establishing the distinction, we first seek to recast quantum mechanics into a classical model which admits either ontic or epistemic states.

Furthermore, the term "hidden variable theory" is commonly used to refer to a particular type of model that posits additional variables alongside the wavefunction. Such theories precisely assume the "realism" we detailed in our discussion of Bell's inequality. However, this term can be confusing because it implies that the wavefunction is already considered real. To avoid this confusion and to encompass a broader range of models, researchers in quantum foundations use the term "ontological model" (82). This term includes models where the wavefunction is not assumed to be real and those where it is the only thing that is real. Though some assume that hidden variable theories necessarily are deterministic, the ontological framework allows for genuine stochasticity in nature. In essence, the term "ontological model" can be equivalent to or more general than a hidden variable theory, depending on the scope of the latter. This "reality" of the quantum state is referred to as ψ-ontology, and theorems that attempt to establish this view are called ψ-ontological theorems. ψ-ontological models of quantum mechanics are models which assume the existence of ontic states in quantum mechanics. Thus, ψ-ontic and ψ-epistemic are both ψ-ontological models of quantum mechanics.

3.1 Prepare and Measure Procedures

Preparation and measurement procedures are lists of instructions for performing quantum experiments in the lab (Harrigan and Spekkens 2). In quantum theory, every preparation P is associated with a density operator ρ in Hilbert space, and every measurement M is associated with a positive operator valued measure (POVM) $\{E_k\}$. The outcome of the measurement is recorded, and the system is then discarded (2). The experimenter can repeat the whole process of preparing and measuring as many times as desired to build up frequency statistics for comparison with the probabilities predicted by some physical theory. The probability of obtaining outcome k in measurement M, given preparation P, is given by the generalised Born rule as (2):

$$\mathrm{p}(k|M, P) = \mathrm{Tr}\left(\rho E_k\right). \tag{2}$$

3.2 ψ-Ontological Models of Quantum Mechanics

As described by Harrigan and Spekkens (2), in an ontological model, a preparation procedure creates a system characterised by certain properties, while a measurement procedure unveils information about these properties. The comprehensive description of a system's properties is termed the ontic state, denoted by λ, with the ontic state space represented by Λ, the set of admissible ontic states (2).

It is important to note that an observer with knowledge of the preparation P might still possess incomplete information about λ. Consequently, the observer may assign a probability distribution $p(\lambda|P)$ over Λ when the preparation is known to be P. In this context, the wavefunction ψ prepared by P_ψ can be described by the probability distribution $p(\lambda|P_\psi)$. Under measurement, the ontic state λ can determine the probability $p(k|\lambda, M)$ of distinct outcomes k for the measurement M (3).

For an ontological model to reproduce the predictions of the operational theory, it must reproduce the probability of k given M and P by the formula (3):

$$\int_\Lambda d\lambda, p(k|M,\lambda)p(\lambda|P) = p(k|M,P). \tag{3}$$

For the model to reproduce quantum statistics, we assume that:

$$\mathrm{p}(k|M,P) = \mathrm{Tr}\left(\rho E_k\right), \tag{4}$$

just as we described the prepare and measure procedures (3). See Appendix 8.5 for a generalisation of the preparation P and the measurement M.

3.3 Classifying Ontological Models

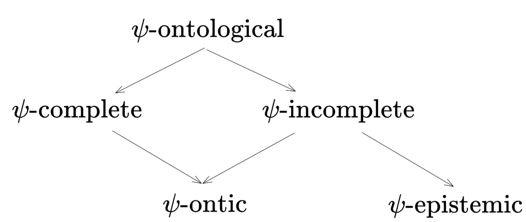

Figure 2: The classification of ψ-ontological models of quantum mechanics. ψ-ontological models can either be ψ-complete or ψ-incomplete. The ψ-complete model is necessarily ψ-ontic, while the ψ-incomplete model is either ψ-ontic or ψ-epistemic.

In the context of ontological models in quantum mechanics, a distinction is made between so-called ψ-complete and ψ-incomplete models. As Harrigan and Spekkens describe (4), an ontological model is considered ψ-complete if its ontic state space Λ is isomorphic to the projective Hilbert space $\mathcal{PH}$, and each preparation procedure P_ψ associated with a given wavefunction ψ in quantum theory is associated with a Dirac delta function centred at the ontic state λ_ψ that is isomorphic to ψ (4):

$$p\left(\lambda|P_\psi\right) = \delta\left(\lambda - \lambda_\psi\right). \tag{5}$$

Such models assign reality to the wavefunction as a physical property of the system.

On the other hand, an ontological model is said to be ψ-incomplete if it is not ψ-complete. This failure could arise due to the presence of additional supplementary variables or because the quantum state does not parameterise the ontic states of the model at all (4).

To further differentiate between such models, a ψ-ontic model is defined as one in which the epistemic states associated with distinct quantum states are completely non-overlapping, i.e., different quantum states pick out disjoint regions of Λ. The wavefunction in such models is a physical property of the "real" state of the system, and obtaining a complete description of reality for the state of the system would allow the wavefunction ψ to be deduced (4).

In contrast, a model is ψ-epistemic if there exist two preparation procedures, P_{ψ_1} and P_{ψ_2}, and a state $\lambda \in \Lambda$ such that the probability of obtaining λ under P_{ψ_1} and P_{ψ_2} is non-zero, indicating an overlap between the two epistemic states (5). This can also be expressed as the ontic state λ being consistent with both quantum states ψ_1 and ψ_2. In a ψ-epistemic model, distinct quantum states can be consistent with the same ontic state, and thus, the quantum state is said to have an epistemic character. It is important to note that the question of interest here is whether pure quantum states have an epistemic character, and not whether the wavefunction is a representation of knowledge in general (for example, contended by the Copenhagen interpretation). Therefore, we use the term ψ-epistemic instead of simply "epistemic". It is also worth noting that any model can be classified as either ψ-complete or ψ-incomplete, and ψ-ontic or ψ-epistemic. However, only three types of models exist, as one of the four combinations represents an empty set. In particular, if a model is ψ-complete, it is also ψ-ontic (5). These concepts are illustrated below:

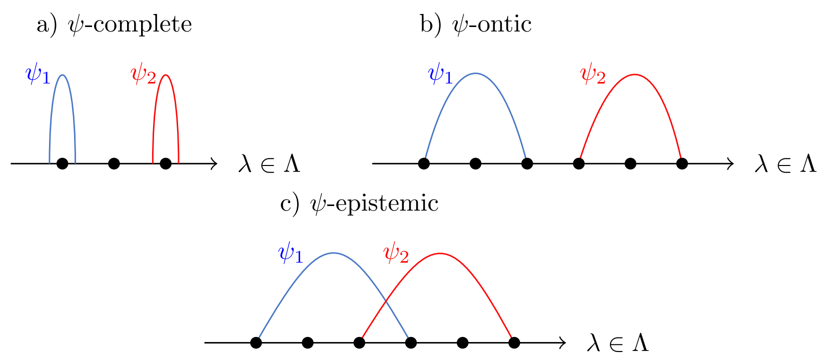

Figure 3: Representation of probability distributions associated with wavefunction ψ over the ontic space Λ for (a) ψ-complete models, (b) ψ-ontic models and (c) ψ-epistemic models. Note that the wavefunction ψ specifies a unique λ in (a), while ψ corresponds to a distribution of λ in (b).

3.4 Examples of ψ-Ontological models

We will discuss two examples of ontological models to make the above concepts concrete. The first example is an ψ-epistemic model and the second being a ψ-complete model. The first model is the Spekkens Toy bit model from developed by Robert Spekkens in 2007 (Leifer 73). The second model is the Beltrametti-Bugajski model. For simplicity, both models are in the two-dimensional Hilbert space.

3.4.1 Spekkens Toy Model

The Spekkens toy model is a discrete variable toy model developed by Robert Spekkens in 2007 (Leifer 73). It assumes the system is always in one of four possible ontic states (x, y), where x and y take values of $+1$ or -1. Spekkens employs the knowledge-balance principle (KCP) restricts the information that can be known about the ontic state to at most half of the time, and measurements must cause a disturbance to the ontic state to satisfy KCP (73).

As described by Leifer (73), the permissible states of maximal knowledge are $|\pm x\rangle, |\pm y\rangle, |\pm z\rangle$. The first two determine whether the values are positive or negative (for the x and y values, respectively). The last determines whether the value of x, y have the same sign, that is, $|+z\rangle$ for $xy = 1$ and $|-z\rangle$ for $xy = -1$. As an example, the permissible ontic states for $|+x\rangle$ are $(+1, +1), (+1, -1)$. The permissible ontic states for $|+y\rangle$ are $(+1, +1), (-1, +1)$. Here, there is an

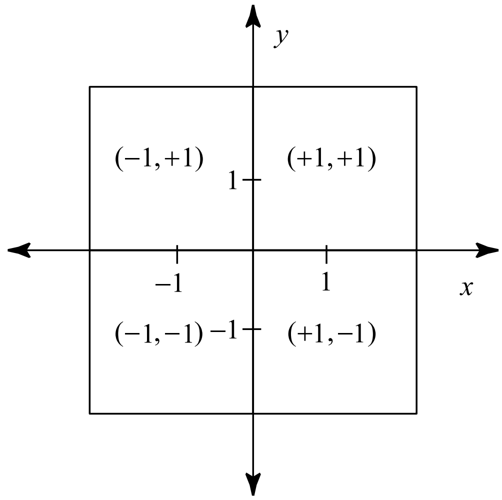

Figure 4: The ontic state space Λ of the Spekkens toy model. Each possible ontic state is labelled as $(\pm 1, \pm 1)$. Adapted from Leifer (73).

overlap of $|+x\rangle, |+y\rangle$ for $(+1, +1)$ (73). Thus, these possible states are epistemic states, as they necessarily overlap with other states.

In this model, measurements cause a random exchange of ontic states, allowing for repeatability while still maintaining uncertainty. For example, measuring $|\pm x\rangle$ will have a 50% chance to change the y value from $+1$ to -1 and vice versa (74). If we were to repeat the measurement, we would still get the same measurement outcome for $|\pm x\rangle$. This ensures that the KCP is satisfied. The model successfully predicts the outcomes of measurements of Pauli observables X, Y, and Z.

The ψ-epistemic model under consideration can be described in terms of the possible preparation and measurement sets P and M, respectively. The preparation set P consists of six elements: $|+x\rangle$, $|-x\rangle$, $|+y\rangle$, $|-y\rangle$, $|+z\rangle$, $|-z\rangle$, and the maximally mixed state $I/2$, where:

$$\begin{aligned}\frac{I}{2} &= \frac{1}{2}|+x\rangle\langle +x| + \frac{1}{2}|-x\rangle\langle -x| \\ &= \frac{1}{2}|+y\rangle\langle +y| + \frac{1}{2}|-y\rangle\langle -y| \\ &= \frac{1}{2}|+z\rangle\langle +z| + \frac{1}{2}|-z\rangle\langle -z|.\end{aligned} \tag{6}$$

The measurement set includes three measurements: $X = \{|+x\rangle, |-x\rangle\}$, $Y = |+y\rangle, |-y\rangle$, and $Z = |+z\rangle, |-z\rangle$. The ontic state space, denoted by Λ, is a finite set of four elements: $(+1, +1)$, $(+1, -1)$, $(-1, +1)$, and $(-1, -1)$. The integral from Equation 3 is replaced by a simple sum over the elements of Λ, given that it is a finite set:

$$\sum_{\lambda \in \Lambda} p(E|M, \lambda)\mu(\lambda) = \mathrm{Tr}(E\rho). \tag{7}$$

Each measurement is associated with a unique conditional probability distribution, which can be easily calculated using the ontic state space. For instance, the conditional probabilities for the X measurement are:

$$\begin{aligned}p(+y|Y, (+1, +1)) &= p(+y|Y, (-1, +1)) = 1 \\ p(+y|Y, (+1, -1)) &= p(+y|Y, (-1, -1)) = 0 \\ p(-y|Y, (+1, +1)) &= p(-y|Y, (-1, +1)) = 0 \\ p(-y|Y, (+1, -1)) &= p(-y|Y, (-1, -1)) = 1.\end{aligned} \tag{8}$$

3.4.2 The Beltrametti-Bugajski model

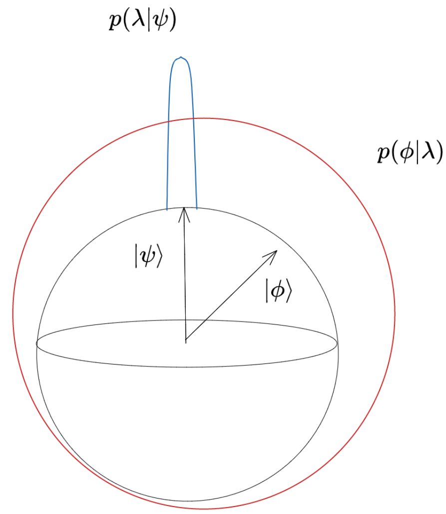

Figure 5: Ontic states in the Beltrametti-Bugajski model. Adapted from Harrigan and Spekkens (6).

The Beltrametti-Bugajski model (Harrigan and Spekkens 6) is a ψ-complete model that provides a thorough rendering of what is commonly referred to as an orthodox interpretation of quantum mechanics. The model posits that the ontic state space Λ is precisely the projective Hilbert space, $\Lambda = \mathcal{PH}$, such that each system prepared in a quantum state ψ with P_ψ is associated with a sharp probability distribution over Λ, denoted as (6):

$$p(\lambda|P_\psi) = \delta(\lambda - \psi), \tag{9}$$

where λ_ψ is some unique ontic state associated with the ψ. The model reproduces quantum statistics by assuming that the probability of obtaining an outcome k of a measurement procedure M depends on the system's ontic state λ, such that (6):

$$p(k|M, \lambda) = \mathrm{Tr}(|\lambda\rangle\langle\lambda|E_k), \tag{10}$$

where E_k is the POVM that associated with M and $|\lambda\rangle \in \mathcal{H}$ denotes the quantum state associated with $\lambda \in \mathcal{PH}$. Then, we know that (6):

$$\begin{aligned} p(k|M, \lambda) &= \int_\Lambda d\lambda, p(k|M, \lambda)p(\lambda, \psi) \\ &= \int_\Lambda d\lambda, p(k|M, \lambda)\delta(\lambda - \lambda_\psi) \\ &= \mathrm{Tr}(|\psi\rangle\langle\psi|E_k), \end{aligned} \tag{11}$$

so we can reproduce the outcomes of quantum mechanics.

Given the above examples of ontological models, we now delve into so called "no-go" theorems of quantum mechanics which impose theoretical and physical restrictions on ontological models beyond the Bell's theorem.

4 Measurement Non-Contextuality and the Kochen-Specker Theorem

Measurement non-contextuality is a property of physical theories, including in classical mechanics and quantum mechanics, which asserts that the outcome of a measurement does not depend on the context of other measurements performed on the same system. In other words, the result of a measurement is independent of which other measurements are being performed concurrently or sequentially. In the context of ontological models, the below figure illustrates a consequence of measurement non-contextuality:

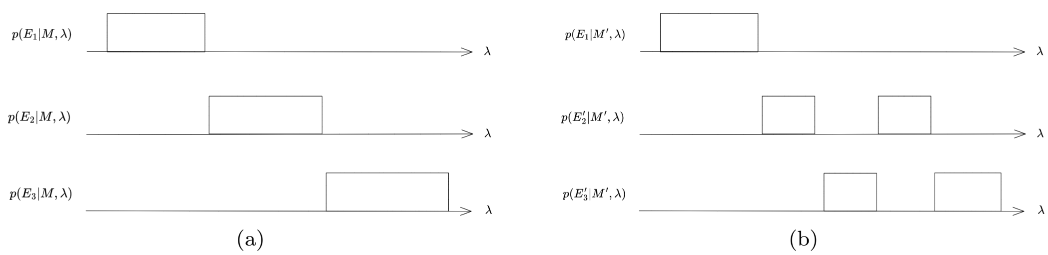

Figure 6: In (a), we measure the POVM E_1, E_2, E_3 associated with the measurement M. In (b), we measure the POVM E_1, E_2', E_3' associated with measurement M'. Under measurement non-contextuality, $p(E_1|M,\lambda) = p(E_1|M',\lambda)$. That is, irrespective of the measurements conducted, the associated probability of finding E_1 for some ontic state λ is always the same.

The Kochen-Specker theorem is a no-go theorem which proves that all ontological models of quantum mechanics in a Hilbert space of dimension greater than or equal to 3 must preserve measurement contextuality. The Kochen-Specker theorem shows that it is impossible to associate definite numerical values of either 1 or 0 with commuting projections in a Hilbert space of dimension greater than or equal to 3 (Peres 175). This implies that any theory that attempts to assign a definite outcome to a quantum measurement must be contextual. That is, the outcome of a measurement cannot be independent of whether it is measured alone or with other observables. Specifically for measurements A, B, C, if $[A, B] = [A, C] = 0$ and $[B, C] \neq 0$, then measuring A alone cannot be equivalent to measuring A together with B or C (175). Thus, measurements must be contextual for ψ-ontological models.

4.1 Kochen-Specker theorem for Three-dimensional Hilbert Space

As described by Peres (175), the theorem's generalised proof proceeds as follows. Let $u_1, \ldots, u_N$ form a complete set of orthonormal vectors. Each matrix $P_m = u_m u_m^\dagger$ is a projection operator on the vector $\boldsymbol{u}_m$. These matrices commute and satisfy $\Sigma P_m = \mathbb{1}$. There exist N ways of associating the value 1 with one of these matrices (and hence one of the vectors u_m), and the value 0 with the remaining $N-1$ matrices. Consider multiple distinct orthogonal bases that may share some of their unit vectors. Assume that if a vector belongs to more than one basis, the value (1 or 0) associated with it is the same regardless of the choice of other basis vectors. In 1967, Kochen and Specker demonstrated a contradiction resulting from this assumption.

In this report, we describe Peres' proof of the Kochen-Specker theorem for the Hilbert space of dimension 3. As described by Peres (175), we have 33 vectors for which squares of direction cosine along the x, y, z axes sum to 1. The given combinations are (176):

$$0+0+1, 0+\frac{1}{2}+\frac{1}{2}, 0+\frac{1}{3}+\frac{2}{3}, \frac{1}{4}+\frac{1}{4}+\frac{1}{2}, \tag{12}$$

and their permutations. The direction cosine for each x, y, z direction of a vector is the component of the vector in some direction over the magnitude of the vector. For example, the direction cosine for some vector v in the x direction is $\frac{v_x}{|v|}$.

The components of the vectors can be $0, 1, \bar{1}, 2, \bar{2}$. 2 denotes $\sqrt{2}$, while the bar denotes a negative component (ex. $\bar{1} = -1$). As an example, $2\bar{1}0$ is the vector $(\sqrt{2}, -1, 0)$. Vectors in opposite directions, like $2\bar{1}0$ and $\bar{2}10$, are counted once.

As Peres argues, these vectors are invariant under interchange of the x, y, z axes (177). Thus, we could arbitrarily assign 1 (first column in below table) and 0 to some of the vectors, as other assignments would be interchanging the axes or reversing them. For an orthogonal set of vector, we only denote one of them to have 1 while the rest is 0. The table from Peres (177) is displayed below:

Orthogonal triad			Other vectors		The first vector is 0 because of:
001	100	010	110	$1\bar{1}0$	choice of z axis
101	$\overline{101}$	010			choice of x vs $-x$
011	$0\bar{1}1$	100			choice of y vs $-y$
$1\bar{1}2$	$\bar{1}12$	110	$\bar{2}01$	021	choice of x vs y
102	$\bar{2}01$	010	$\bar{2}11$		orthogonality to second and third vector
211	$0\bar{1}1$	$\bar{2}11$	102		orthogonality to second and third vector
201	010	$\overline{102}$	$\overline{112}$		orthogonality to second and third vector
112	$1\overline{10}$	112	0201		orthogonality to second and third vector
012	100	$0\bar{2}1$	$1\bar{2}1$		orthogonality to second and third vector
121	$\bar{1}01$	$1\bar{2}1$			orthogonality to second and third vector

Note that the additional vector in the columns after the first is orthogonal to the vector in the first column. We see $100, 021, 0\bar{1}2$ are all denoted as 0. However, these vectors are orthogonal (176). This is a contradiction, as we require each set of vectors to include one vector denoted as 1. Thus, we have proved the Kochen-Specker theorem for the Hilbert space of dimension 3, though similar thinking can help us extend this result to higher dimensions.

In conclusion, the Kochen-Specker theorem is a powerful result that has profound implications for the foundations of quantum mechanics. It shows that any attempt to construct an ontological model of quantum mechanics that assigns definite values to all observables necessarily has measurement contextuality. In other words, the outcome of a measurement in quantum mechanics cannot be independent of whether it is measured alone or with other observables. The theorem has been proven for Hilbert spaces of dimension greater than or equal to 3 and provides a clear example (in addition to Bell's theorem) of the mathematical restrictions on possible ontological models of quantum mechanics. We now examine the PBR theorem.

5 Pusey-Barrett-Rudolph Theorem

The Pusey-Barrett-Rudolph (PBR) theorem is a significant result in the field of quantum foundations that was proposed in 2012 by Matthew Pusey, Jonathan Barrett, and Terry Rudolph. In their work, Pusey, Barrett, and Rudolph presented a no-go theorem that reveals a contradiction between the predictions of quantum theory and ψ-epistemic models (Pusey et al. 1).

Their main result is that if two distinct quantum states, $|\psi_1\rangle$ and $|\psi_2\rangle$, have overlapping ontic state distributions $\mu_1(\lambda) = p(\lambda|P_{\psi_1})$ and $\mu_2(\lambda) = p(\lambda|P_{\psi_2})$, then there is a contradiction with the predictions of quantum theory. The intersection of their supports (shared ontic states), denoted as Δ, must have non-zero measure for this contradiction to occur. Initially, they presented a simple version of the argument that only works when $|\langle\psi_1|\psi_2\rangle| = 1/\sqrt{2}$. However, they then extended the argument to arbitrary $|\psi_1\rangle$ and $|\psi_2\rangle$, and ultimately presented a more formal version that can account for experimental error and noise (1). Here, we consider a special case of the theorem as described by Pusey et al., which elucidates the thought process behind their general theorem.

As described by Pusey et al. (2), suppose we have preparing two quantum systems independently, where each method corresponds to a specific quantum state: $|\psi_1\rangle$ and $|\psi_2\rangle$. We can choose a basis for the Hilbert space such that $|\psi_1\rangle, |\psi_2\rangle \in \{|0\rangle, |+\rangle\}$. If the probability distributions of the physical states that prepare these two quantum states overlap, then there exists a region Δ where a physical state λ can result in either quantum state with probability $q > 0$ (2).

Consider the case where Alice and Bob independently prepare the quantum states $|\psi_1\rangle, |\psi_2\rangle$. The physical states of the two systems are uncorrelated, meaning the preparation of one system does not affect the preparation of the other (2). If there exists a physical state λ_1 prepared by the Alice and a physical state λ_2 prepared by Bob, such that both of these physical states lie in the overlap region Δ, then the physical state of the combined system is compatible with any of the four possible quantum states $|00\rangle$, $|0+\rangle$, $|+0\rangle$, and $|++\rangle$. Pusey et al. makes the assumption that there exists some region Δ compatible with all four statevectors (2).

After preparing two independent quantum systems in either state $|0\rangle$ or $|+\rangle$, the distributions $\mu_1(\lambda)$ and $\mu_2(\lambda)$ are assumed to overlap. This implies that the preparation of either quantum state results in a λ from the overlap region Δ with probability at least q. When the two systems are brought together, say to Charlie, and he performs a measurement on the two qubits, he chooses the measurement such that the following four possible outcomes are observed (3):

$$\begin{aligned}
|\xi_1\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \\
|\xi_2\rangle &= \frac{1}{\sqrt{2}}(|0-\rangle + |1+\rangle), \\
|\xi_3\rangle &= \frac{1}{\sqrt{2}}(|+1\rangle + |-0\rangle), \\
|\xi_4\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle),
\end{aligned} \tag{13}$$

where the first state $|\xi_1\rangle$ is orthogonal to $|00\rangle$, and the subsequent states are orthogonal to $|0+\rangle, |+0\rangle, |++\rangle$ respectively.

However, the probabilities of each outcome are zero for a corresponding preparation of $|\psi_1\rangle$ and $|\psi_2\rangle$. This leads to a contradiction, as the measuring device is uncertain which preparation method was used with probability q^2 in our epistemic model. However, for our physical measurement, we know that we can associate each measurement outcome with only three statevectors. Thus, there does not exist some region Δ compatible with all four statevectors (3). This logic informs the general PBR theorem.

In the general case (3), the PBR theorem states that for any non-orthogonal states $|\psi_1\rangle$ and

$|\psi_2\rangle$, we can choose some basis $|a\rangle, |b\rangle$ where:

$$\begin{aligned} |\psi_1\rangle &= \cos\frac{\theta}{2}|a\rangle + \sin\frac{\theta}{2}|b\rangle, \\ |\psi_2\rangle &= \cos\frac{\theta}{2}|a\rangle - \sin\frac{\theta}{2}|b\rangle, \end{aligned} \tag{14}$$

where $0 < \theta < \frac{\pi}{2}$. Intuitively, we can think of this within the Bloch sphere picture. We can always find a plane on the Bloch sphere which is parallel to both $|\psi_1\rangle, |\psi_2\rangle$. Then, we can necessarily choose orthogonal bases $|a\rangle, |b\rangle$ on this plane which satisfy the above equation, where $|\psi_1\rangle, |\psi_2\rangle$ are not orthogonal. Using the above construction, Pusey et al. demonstrate (5) that we can always perform some quantum circuit procedure which rejects the notion that any quantum state we select is ψ-epistemic.

In summary, the PBR theorem presents a no-go result that indicates the impossibility of ψ-epistemic models in reproducing quantum statistics. This result is analogous to Bell's theorem, which shows that local theories cannot reproduce the predictions of quantum theory under certain assumptions.

6 Conclusion

In conclusion, this report has delved into various aspects of the foundations of quantum mechanics, ranging from Bell's inequality to the Pusey-Barrett-Rudolph theorem. Through our exploration, we have learned about the limitations of ontological models and how they challenge our understanding of reality. The no-go theorems we have explored have demonstrated the limitations of ontological models and challenged us to think beyond our preconceived notions of reality. Yet, through mathematical exploration and formalization, we have gained a powerful toolbox for investigating the foundations of quantum mechanics. As we continue to push the boundaries of our understanding, we are forced to confront the strange and often counter-intuitive implications of quantum mechanics.

7 Bibliography

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8 Appendix

8.1 Postulates of Quantum Mechanics

We will discuss the three postulates of quantum mechanics below, as adapted from Chapter 2.2 from Nielsen and Chuang (80):

(Postulate 1) Hilbert space: The state of a quantum mechanical system is described by a vector in a complex Hilbert space $\mathcal{H}$. The Hilbert space is a mathematical space with some special properties that allow us to describe the behavior of quantum particles. For example, we can use the Hilbert space to represent the position and momentum of a particle, or the spin of an electron. The Hilbert space is a complete space, meaning that it contains all possible states of a quantum system. We will be using Dirac notation to denote vectors in the Hilbert space. Dirac notation is a common notation used in quantum mechanics to represent quantum states and operators. It was introduced by British physicist Paul Dirac in the 1930s and has since become a standard way of expressing quantum mechanics. The notation uses a ket vector, represented by the symbol $|\psi\rangle$, to represent a quantum state, and a bra vector, represented by the symbol $\langle\psi|$, to represent the conjugate transpose of the ket vector. These belong to the Hilbert space, which is an inner product space. That is, the operation $\langle\psi'|\psi\rangle$. See Appendix 8.2 for more info.

(Postulate 2) Measurement and Born rule: When a measurement is made on a quantum system, the result is one of the eigenvalues of the hermitian measurement operator M. The probability of obtaining each eigenvalue m_i is given by the Born rule:

$$p(m_i) = |\langle\psi|\psi_i\rangle|^2, \tag{15}$$

where $|\psi_i\rangle$ is the corresponding eigenvector of M, and $|\psi\rangle$ is the state vector of the quantum system. After the measurement, the state of the system collapses to the corresponding eigenvector $|\psi_i\rangle$:

$$|\psi\rangle \rightarrow \frac{P_i|\psi\rangle}{\sqrt{\langle\psi|P_i|\psi\rangle}}, \tag{16}$$

where P_i is the projection operator onto the subspace spanned by the eigenvector $|\psi_i\rangle$.

(Postulate 3) Time evolution and Schrödinger equation: The time evolution of a quantum mechanical system is described by the Schrödinger equation, which is a linear partial differential equation that describes how the state vector changes over time. The Schrödinger equation is typically written as:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{17}$$

where $|\psi(t)\rangle$ is the state vector at time t, H is the Hamiltonian operator, and $\hbar$ is the reduced Planck constant.

These postulates provide a framework for understanding the behaviour of quantum mechanical systems, and have been shown to accurately predict the results of experiments. For our purposes, we could consider an equally valid description of the postulates in terms of pure and mixed states. In general, pure states are simple the outer products of the statevector, that is:

$$\rho = |\psi\rangle\langle\psi|, \tag{18}$$

while mixed states are a statistical ensemble of pure states. It is of the form:

$$\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|, \tag{19}$$

where p_i is the probability for the mixed state to be in the corresponding pure state. The postulates of quantum mechanics can be rewritten in terms of pure and mixed states. (See Nielsen and Chuang, pg 102, for more complete description). Importantly, for a collection of measurement operators $\{M_m\}$ where the outcome m corresponds to the operator M_m, the probability of measure m for the pure or mixed state ρ is given as:

$$p(m) = \text{Tr}(M_m^\dagger M_m\rho). \tag{20}$$

This notation will be used in the mathematical descriptions of the ontological models.

8.2 Dirac Notation

Explicitly, the ket $|\psi\rangle$ will have the vector representation:

$$|\psi\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{bmatrix}, \tag{21}$$

where each element denotes the components of the statevector in some orthonormal basis, like $|0\rangle, |1\rangle, \ldots, |n\rangle$. The components of the statevector are complex numbers, and the sum of absolute square of the components equals 1. The conjugate transpose of the state vector has the vector representation:

$$\langle\psi| = \begin{bmatrix} \psi_1^* & \psi_2^* & \ldots & \psi_n^* \end{bmatrix}. \tag{22}$$

The inner product is the multiplication of the bra and the ket. For example, given:

$$|\psi\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}, \tag{23}$$

we know that:

$$\langle\psi|\psi\rangle = \begin{bmatrix} \psi_1^* & \psi_2^* \end{bmatrix} \times \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \psi_1^*\psi_1 + \psi_2^*\psi_2 = 1. \tag{24}$$

The outer product is the multiplication of the ket and the bra. For example, given:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{25}$$

we know that:

$$|0\rangle\langle 0| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \times \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{26}$$

For a more comprehensive description, see https://www.youtube.com/watch?v=2HJSf-kkN1U. Additionally, see https://quantum.phys.cmu.edu/QCQI/qitd114.pdf

8.3 EPR Theorem

Alice and Bob both apply the measurement M. Let's assume that there exists some basis in which the measurement M has the spectral decomposition:

$$(+1)|\psi\rangle\langle\psi| + (-1)|\psi'\rangle\langle\psi'|, \tag{27}$$

and that the standard basis had the decompositions:

$$\begin{aligned} |0\rangle &= \alpha|\psi\rangle + \beta|\psi'\rangle \\ |1\rangle &= \gamma|\psi\rangle + \delta|\psi'\rangle, \end{aligned} \tag{28}$$

then the bell state would have the decomposition:

$$\frac{(\alpha\delta - \gamma\beta)|\psi\psi'\rangle + (\beta\gamma - \delta\alpha)|\psi'\psi\rangle}{\sqrt{2}} = (\alpha\delta - \gamma\beta)\frac{|\psi\psi'\rangle - |\psi'\psi\rangle}{\sqrt{2}}, \tag{29}$$

from which we conclude that the measurement M will give orthogonal eigenstates. Thus, Alice's measurement of $+1$ implies that Bob will measure -1, and vice versa.

8.4 Bell's theorem

The below section is the proof of Bell's theorem as described by Nielsen and Chuang (115).

According to Nielsen and Chuang (115), we can observe the expectation value of the quantity $QS+RS+RT-QT$. Since $QS+RS+RT-QT = (Q+R)S+(Q-R)T$, then for all combinations of $Q, R \in \{-1, +1\}$, we know that either $Q+R = 0$ or $Q-R = 0$. Thus, we know that the maximum and minimum values of $(Q+R)S+(Q-R)T$ are $+2, -2$ respectively.

We suppose that the probability $p(q, r, s, t)$ is the probability that the physical properties Q, R, S, T have values $q, r, s, t \in \{-1, +1\}$, possibly due to measurement preparation and environmental noise. We are allowed to make such an assumption, as physical properties have observer independent values. If $E(\cdot)$ denotes the expectation value of some quantity, then we know that:

$$\begin{aligned} E(QS+RS+RT-QT) &= \sum_{q,r,s,t} p(q,r,s,t)(qs+rs+rt-qt) \\ &\leq \sum_{q,r,s,t} 2p(q,r,s,t) \\ &= 2\sum_{q,r,s,t} p(q,r,s,t) = 2. \end{aligned} \tag{30}$$

Likewise, the expectation value of a sum is the sum of expectation values, so we can also write:

$$E(QS+RS+RT-QT) = E(QS)+E(RS)+E(RT)-E(QT), \tag{31}$$

so that:

$$E(QS)+E(RS)+E(RT)-E(QT) \leq 2. \tag{32}$$

This is known as the CHSH inequality (Nielsen and Chuang 116). In an experimental context, Charlie can prepare the same state multiple times, and send the two qubits to Alice and Bob. Alice and Bob can repeat the measurements to get the frequency statistics of the physical properties. Thus, the CHSH inequality seems to state that under our assumptions, such a measurement will always lead to the above inequality.

Notably, we have made two definite assumptions here. The first is that P_Q, P_R, P_S, P_T are physical properties with definite values Q, R, S, T. The second is that Alice's measurement does not affect Bob's measurement. The second assumption is the principle of locality (Nielsen and Chuang 117).

However, the above example is easily refuted within quantum mechanics. Like above, Charlie prepares the bell state:

$$\psi = \frac{|01\rangle - |10\rangle}{\sqrt{2}}. \tag{33}$$

The first qubit is again given to Alice, and the second qubit is given to Bob. If we carefully choose Alice's measurements as:

$$Q = Z_1, \; R = X_1, \tag{34}$$

and Bob's measurement as:

$$S = \frac{-Z_2 - X_2}{\sqrt{2}}, \; T = \frac{Z_2 - X_2}{\sqrt{2}}. \tag{35}$$

Using these values, we calculate the expectation values to be:

$$E(QS) = \frac{1}{\sqrt{2}}, E(RS) = \frac{1}{\sqrt{2}}, E(RT) = \frac{1}{\sqrt{2}}, E(QT) = -\frac{1}{\sqrt{2}}, \tag{36}$$

for which:

$$E(QS)+E(RS)+E(RS)-E(QT) = 2\sqrt{2}, \tag{37}$$

which violates the CHSH inequality.

8.5 Generalised Preparation and Measurement

As described by Leifer (83), a quantum system's preparation in density operator state ρ corresponds to its occupation of an ontic state $\lambda \in \Lambda$ (λ is an ontic state, while Λ is the set of possible ontic states). However, the preparation procedure may not determine λ exactly, so our knowledge of λ is described by a probability measure μ over the measurable space Λ, with a σ-algebra Σ and a σ-additive function $\mu : \Sigma \to [0, 1]$ satisfying $\mu(\Lambda) = 1$. The preparation of mixed states may result in different probability measures over the ontic states, leading to preparation contextuality. A quantum state ρ is associated with a set Δ_ρ of probability measures rather than a single unique measure (82)

As described by Leifer (83), a measurement $M \in M$ may depend on λ only probabilistically, either because nature is fundamentally stochastic or because the measuring device's response depends on degrees of freedom within the measuring device beyond the experimenter's control. Each POVM M is represented by a conditional probability distribution $\Pr(E|M, \lambda)$ over M, where $\Pr(E|M, \lambda) \geq 0$ for all $E \in M$ and $\sum_{E \in M} \Pr(E|M, \lambda) = 1$ for any fixed λ. To calculate the model's predicted probabilities of observing a particular outcome, we must average over our ignorance about λ, where $\Pr(E|M, \lambda)$ is a measurable function of λ.