Can the universe be in a mixed state?

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Abstract
It has been proposed that the universe is in a mixed state or its quantum state is an impure density matrix, not a wave function. In this paper, I argue that this view can hardly be consistent with the latest results about the reality of the wave function.

Quantum mechanics with a fundamental density matrix (W-QM) has been proposed and discussed recently (Diér et al., 2005; Maroney, 2005; Chen, 2018, 2019, 2020). It replaces the wave function in quantum mechanics with the density matrix and correspondingly the Schrödinger equation with the von Neumann equation. According to these authors, W-QM and QM are empirically equivalent. Moreover, since quantum dynamics can be formulated directly in terms of the density matrix $W$, it is reasonable to assume that $W$ represents something objective, and the ontic state of the universe is represented by an impure density matrix, not by a wave function. This view has been called density matrix realism (Chen, 2018). In this paper, I will argue that this view can hardly be consistent with the latest results about the reality of the wave function. In particular, I will argue that when assuming an ontological models framework and preparation independence, there is no density matrix realism for W-QM. The reason is simple: we can prove $\psi$-ontology under these assumptions, and since $\psi$-ontology and W-ontolgy are incompatible, this will exclude density matrix realism. Finally, I will also discuss possible ways to avoid this result for density matrix realists.

QM and W-QM, in a minimum formulation, are two empirically equivalent algorithms for calculating probabilities of measurement results. We can assign a wave function or an impure density matrix to the universe (or any isolated subsystem of it) and use either QM or W-QM for empirical predictions. Before my analysis, I will first clarify two things, ignorance of which may often mislead researchers. First, the issue is to determine
whether the wave function is real in QM or the impure density matrix is real in W-QM. It is irrelevant to whether an impure density matrix may be real in QM or whether a subsystem of the universe can also have a wave function and whether the wave function is real in W-QM etc. According to the proponents of density matrix realism, W-ontology excludes ψ-ontology; this is clear when the wave function is complete in QM and the impure density matrix is complete in W-QM such as in many worlds theory, and it is also true when there are hidden variables such as for BM and W-BM. Next, the reality of the wave function or the impure density matrix is more than their objectivity. Reality here means that the wave function or the impure density matrix is a description of the ontic state of a single system, while objectivity also permits that they are only properties of a statistical ensemble, not properties of a single system. Thus, reality implies objectivity, but the opposite is not true.

In recent years, a general and rigorous approach called ontological models framework (OMF) has been proposed to determine the underlying ontology of a quantum algorithm (Harrigan and Spekkens 2010; Pusey, Barrett and Rudolph, 2012; Leifer, 2014). We will use this framework to analyze the reality of the wave function in QM and the reality of the impure density matrix in W-QM.\footnote{It seems that there is also a possibility that both W-ontology and ψ-ontology are true. In other words, the complete ontic state of a system includes both its wave function in QM and its mixed state in W-QM. But this is not the case that density matrix realists usually considered, and I will not consider this possibility either. In this case, W-ontology will be useless to solve the puzzles of the arrow of time etc.}

The framework has two fundamental assumptions. Below is a formulation of these assumptions applicable to both QM and W-QM.

The first assumption of OMF is about the existence of the underlying state of reality. It says that when QM assigns a wave function or W-QM assigns a density matrix to a physical system\footnote{This means that the result will rely on the ontological models framework, and one may avoid the result by rejecting one or more assumptions of the framework (see later discussion). I will not consider the possibility that reality of something can only be assumed and the assumption rejects examination and test.}, the system has a well-defined set of physical properties or an underlying ontic state, which is usually represented by a mathematical object, \( \lambda \). In general, for an ensemble of identically prepared systems, the ontic states of different systems in the ensemble may be different, and the wave function in QM or the density matrix in W-QM corresponds to a probability distribution \( p(\lambda|P) \) over all possible ontic states when the preparation is known to be \( P \), where \( \int d\lambda p(\lambda|P) = 1 \).

The second assumption of OMF is a rule of connecting the underlying ontic states with measurement results, which says that when a measurement

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\( p(\lambda|P) = 1 \)

\footnote{Note that since QM and W-QM are two empirically equivalent algorithms, density matrix realists cannot deny that a physical system can be assigned to a wave function by QM or prepared in a pure quantum state in QM, and similarly, wave function realists cannot deny that a physical system can be assigned to a mixed state by W-QM or prepared in a mixed state in W-QM either.}
is performed, the behaviour of the measuring device is determined by the
ontic state of the system, along with the physical properties of the measuring
device. For example, for a projective measurement $M$, the ontic state $\lambda$ of
a physical system determines the probability $p(k|\lambda, M)$ of different results
$k$ for the measurement $M$ on the system. The consistency with QM or W-
QM then requires the following relation: $\int d\lambda p(k|\lambda, M) p(\lambda|P) = p(k|M, P)$,
where $p(k|M, P)$ is the Born probability of $k$ given $M$ and $P$.

So far, no $W$-ontology theorem has been proved by combining OMF and
W-QM. However, several $\psi$-ontology theorems have been proved by combin-
ing OMF and QM (Pusey, Barrett and Rudolph, 2012; Colbeck and Renner,
2012, 2017; Hardy, 2013), the strongest one of which is the Pusey-Barrett-
Rudolph theorem or the PBR theorem (Pusey, Barrett and Rudolph, 2012).
The PBR theorem shows that when assuming independently prepared sys-
tems have independent ontic states in OMF, the ontic state of a physical
system uniquely determines its wave function, and thus the wave function
of a physical system directly represents the ontic state of the system. This
auxiliary assumption is called preparation independence assumption.

The basic proof strategy of the PBR theorem is as follows. Assume
there are $N$ nonorthogonal states $\psi_i$ ($i=1, \ldots, N$), which are compatible
with the same ontic state $\lambda$.

The ontic state $\lambda$ determines the probability $p(k|\lambda, M)$ of different results $k$ for the measurement $M$. Moreover, there is a
normalization relation for any $N$ result measurement: $\sum_{i=1}^{N} p(k_i|\lambda, M) = 1$.
Now if an $N$ result measurement satisfies the condition that the first state
gives zero Born probability to the first result and the second state gives zero
Born probability to the second result and so on, then there will be a relation
$p(k_i|\lambda, M) = 0$ for any $i$, which leads to a contradiction.

The task is then to find whether there are such nonorthogonal states and
the corresponding measurement. Obviously there is no such a measurement
for two nonorthogonal states of a physical system, since this will permit them
to be perfectly distinguished, which is prohibited by QM. However, such a
measurement does exist for four nonorthogonal states of two copies of a
physical system. The four nonorthogonal states are the following product
states: $|0\rangle \otimes |0\rangle$, $|0\rangle \otimes |+\rangle$, $|+\rangle \otimes |0\rangle$ and $|+\rangle \otimes |+\rangle$, where $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. The corresponding measurement is a joint measurement of the two systems,
which projects onto the following four orthogonal states:

\footnote{It can be readily shown that different orthogonal states correspond to different ontic
states in OMF. Thus the proof given here concerns only nonorthogonal states.}
\[ \phi_1 = \frac{1}{\sqrt{2}} (|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle), \]
\[ \phi_2 = \frac{1}{\sqrt{2}} (|0\rangle \otimes |\rangle - |1\rangle \otimes |\rangle), \]
\[ \phi_3 = \frac{1}{\sqrt{2}} (|+\rangle \otimes |1\rangle + |\rangle \otimes |0\rangle), \]
\[ \phi_4 = \frac{1}{\sqrt{2}} (|+\rangle \otimes |\rangle - |\rangle \otimes |+\rangle), \] (1)

where \( |\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \). This proves that the four nonorthogonal states are ontologically distinct. In order to further prove the two nonorthogonal states \(|0\rangle\) and \(|+\rangle\) for one system are ontologically distinct, the preparation independence assumption is needed. Under this assumption, a similar proof for every pair of nonorthogonal states can also be found, which requires more than two copies of a physical system (see Pusey, Barrett and Rudolph, 2012 for the complete proof).

As noted before, QM and W-QM are two quantum algorithms for calculating probabilities of measurement results, and we can assign a wave function or an impure density matrix to the universe or an isolated subsystem of the universe and use either QM or W-QM for empirical predictions. Now, when combining with OMF, a general framework used to analyze the underlying ontology of a quantum algorithm, we have a \(\psi\)-ontology theorem, the PBR theorem, which shows that the ontic state of a physical system that can be assigned to a wave function uniquely determines its wave function (when assuming two systems being in a product state have independent ontic states). Then, given that the wave function has the same physical meaning, especially the same relationship with the underlying ontic state, for every system that can be assigned to a wave function, it is arguable that the PBR result applies to the universe as a whole, as well as an isolated subsystem of the universe. Thus, different wave functions of the universe will correspond to different ontic states, or in other words, the ontic state of the universe is represented by a wave function.

Certainly, if we have a \(W\)-ontology theorem which shows that the ontic state of a physical system that can be assigned to an impure density matrix uniquely determines the density matrix, then given that the density matrix has the same physical meaning for every system that can be assigned to a density matrix, it is arguable that the result will also apply to the universe as a whole, as well as to an isolated subsystem of the universe. However, due to the existence of the \(\psi\)-ontology theorem, we cannot have such a

\[ \frac{5}{\text{The universe as a whole is a perfectly isolated system. If a density matrix has different meanings for an isolated subsystem of the universe and the universe itself in W-QM, then we cannot know the relation between the impure density matrix assigned to the universe and the ontic state of the universe with the help of experience; we can only measure the subsystems of the universe, and we cannot measure the universe as a whole. The argument is the same for the wave function in QM.}} \]
W-ontology theorem under the same auxiliary assumption in OMF; they contradict each other.

The above result is obvious for a universe being in a product state. Suppose the universe contains an isolated subsystem \( A \) and its environment \( B \) at a given instant. QM will assign two wave functions \( \psi_A \) and \( \psi_B \) to \( A \) and \( B \), and the whole universe is in a product state \( \psi_A \psi_B \). While W-QM will assign two density matrices \( W_A \) and \( W_B \) to \( A \) and \( B \), and the whole universe is in a product state \( W_A W_B \), which is an impure density matrix according to density matrix realism. Now, by the PBR theorem, a \( \psi \)-ontology theorem, the ontic state of each subsystem uniquely determines its wave function (when assuming they have independent ontic states in OMF), and thus the ontic state of the universe also uniquely determines its wave function. In other words, the ontic state of the universe is represented by a wave function. This is inconsistent with density matrix realism, which says that the ontic state of the universe is represented by an impure density matrix, not by a wave function.

For a universe being in an entangled state, it will be useful to analyze the effective wave functions of the subsystems of the universe in order to understand the above result. Take Chen’s (2018) initial projection hypothesis as an example. According to this hypothesis, the initial impure density matrix assigned to the universe by W-QM is the normalized projection operator onto the Past Hypothesis subspace, a special low-dimensional Hilbert space, namely

\[
W_0 = \frac{1}{N} \sum_{i=1}^{N} |\psi_i\rangle \langle \psi_i|,
\]

where \( N \) is the dimension of the Hilbert space, and \( |\psi_i\rangle \) is a set of orthogonal states in the Hilbert space. Correspondingly, QM may assign any wave function in the Hilbert space to the universe at the initial instant (with the same probability). In other words, this impure density matrix is compatible with all wave functions in the Hilbert space. This is just the key idea of Chen (2018) to account for the Past Hypothesis by defining a natural initial condition of the universe; the initial impure density matrix is simple and unique, while there are infinitely many different choices of initial wave functions.\(^8\)

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\(^6\)Since QM and W-QM are considered as universal laws of nature, it is arguable that they apply to any possible universe, not only to our universe.

\(^7\)Note that density matrix realism does not require that the density matrix of every isolated subsystem of the universe is also impure. In other words, wave functions may emerge at the subsystem level in W-QM (Chen, 2019). However, the density matrix of every isolated subsystem of the universe cannot be all pure. In this example, one of \( W_A \) and \( W_B \) must be impure; otherwise the whole density matrix \( W_A W_B \) will be pure, and W-QM will become QM.

\(^8\)If this initial impure density matrix in W-QM uniquely determined the initial wave
Now consider the universes being in two different initial wave functions in Bohmian mechanics, a realist formulation of QM (Goldstein, 2017). Let $A$ be a subsystem of the universe including $N$ particles with position variables $x = (x_1, x_2, ..., x_N)$. Let $y = (y_1, y_2, ..., y_M)$ be the position variables of all other particles in the environment $B$. The two initial wave functions evolve to the following two wave functions at a later instant:

\[
\Psi_1(x, y) = \varphi_1(x)\phi(y) + \Theta(x, y),
\]

\[
\Psi_2(x, y) = \varphi_2(x)\phi(y) + \Theta(x, y),
\]

where $\phi(y)$ and $\Theta(x, y)$ are functions with macroscopically disjoint supports, and the position variables of the particles of $B$ lies within the support of $\phi(y)$.

This means that $\varphi_1(x)$ and $\varphi_2(x)$ (up to a multiplicative constant) are $A$’s two effective wave functions. An effective wave function obeys a Schrödinger dynamics of its own and also satisfies the Born rule, and it is the Bohmian analogue of the usual wave function in QM. Thus the PBR theorem applies to the effective wave functions. Then, the two effective wave functions, $\varphi_1(x)$ and $\varphi_2(x)$, will correspond to two different ontic states. Moreover, since the other terms in the composition of the two universal wave functions $\Psi_1(x, y)$ and $\Psi_2(x, y)$ are the same, these two wave functions also correspond to two different ontic states. However, since these two wave functions in QM are compatible with the same impure density matrix in W-QM (which evolves from the initial impure density matrix $W_0$ by the von Neumann dynamics), and the same impure density matrix represents the same ontic state of the universe according to density matrix realism, there is a contradiction. In other words, density matrix realism is inconsistent with the PBR result.

There are three possible ways to avoid the result of the PBR theorem. The first way is to deny the first assumption of OMF, namely denying that when QM assigns a wave function or W-QM assigns a density matrix to a physical system, the system has a well-defined set of physical properties or an underlying ontic state. This assumption is indeed rejected by QBism (Fuchs et al, 2014) and other pragmatist approaches to quantum theory (Healey, 2017). However, this assumption is necessary for density matrix realism, since if there are no any underlying ontic states, then it will be meaningless to claim that the impure density matrices describe them.

The second way to avoid the result of the PBR theorem is to deny the second assumption of OMF, namely denying that when a measurement is performed on a system, the behaviour of the measuring device, especially

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9 Here it is supposed that the positions of all particles are the same for the two situations.
the probability of different results for the measurement, is determined by the ontic state of the system, along with the physical properties of the measuring device. Note that this assumption is needed for investigating whether an ontological model such as density matrix realism is consistent with the empirical predictions of a quantum algorithm such as W-QM. If this assumption is dropped, then it seems that we cannot know the relation between the impure density matrix assigned to the universe and the ontic state of the universe with the help of experience, and thus we cannot have empirical justification for accepting density matrix realism.

The third way to avoid the result of the PBR theorem is to deny the preparation independence assumption. Although this assumption seems very natural, it is rejected by some \( \psi \)-epistemic ontological models (Lewis et al, 2012). However, even if rejecting this auxiliary assumption, one can also prove that different orthogonal states correspond to different ontic states based on the two fundamental assumptions of OMF (Leifer, 2014). This result is still inconsistent with density matrix realism. For instance, in the above example, the initial impure density matrix \( W_0 \) is also compatible with two orthogonal effective wave functions \( \varphi_1(x) \) and \( \varphi_2(x) \), and thus the inconsistency also exists.

To sum up, I argue that when assuming the ontological models framework and preparation independence, the PBR theorem implies that even though one can assign an impure density matrix to the universe and make empirical predictions using W-QM, the ontic state of the universe is represented by a wave function, not by an impure density matrix. This is against density matrix realism. It remains to see whether any way of avoiding this result, such as rejecting the second assumption of the ontological models framework, is satisfactory for density matrix realists.

References


