# On the Role of Density Matrices in Bohmian Mechanics

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**Abstract**

It is well known that density matrices can be used in quantum mechanics to represent the information available to an observer about either a system with a random wave function ("statistical mixture") or a system that is entangled with another system ("reduced density matrix"). We point out another role, previously unnoticed in the literature, that a density matrix can play: it can be the "conditional density matrix," conditional on the configuration of the environment. A precise definition can be given in the context of Bohmian mechanics, whereas orthodox quantum mechanics is too vague to allow a sharp definition, except perhaps in special cases. In contrast to statistical and reduced density matrices, forming the conditional density matrix involves no averaging. In Bohmian mechanics with spin, the conditional density matrix replaces the notion of conditional wave function, as the object with the same dynamical significance as the wave function of a Bohmian system.

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## 1 Introduction

We wish to dedicate this work to the memory of Jim Cushing, our friend, coworker and colleague.

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In this paper we shall be concerned with the following claim: Once we deal with particles with spin in Bohmian mechanics, we are more or less obliged to regard the quantum state of any system (except the universe) as given by a density matrix, which then has precisely the same dynamical significance as the wave function. The aim of this paper is to elaborate on this statement, as it is far from obvious in what sense a density matrix could represent the dynamical state of a Bohmian system. In fact, our statement is in sharp contrast with that of Bell [2]:

> So in the de Broglie–Bohm theory a fundamental significance is given to the wave function, and it cannot be transferred to the density matrix.

Although this is correct for spin 0 particles, the situation changes as soon as we consider spin or any other internal degree of freedom. To appreciate this point, it is essential to distinguish between different roles that density matrices can play in Bohmian mechanics (or, for that matter, in other versions of quantum mechanics). In one of these roles, the density matrix is of a purely epistemic character, i.e., it expresses ignorance, whereas in another role, a role that has as yet not been discussed in the literature and of which Bell was obviously not aware, a density matrix is of direct significance to the Bohmian particle motion, as the "conditional density matrix."

We distinguish in this paper five roles of density matrices: the statistical, reduced, combined (reduced statistical), conditional, and fundamental density matrix. We explain the relations between them and their relevance to the particle motion. We explain in particular the new notion of conditional density matrix and its relevance to Bohmian mechanics.

A particular consequence of our discussion is that the same system can, at one and the same time, have a conditional density matrix and, say, a different reduced density matrix. Thus, when speaking about "the" density matrix of a system, it is necessary to specify whether one refers to the reduced or the conditional density matrix. This is new: among the traditional types of density matrices, it is always clear (except for the ambiguity in some cases as to whether one should consider collapsed or uncollapsed wave functions) which type of density matrix is relevant to a given system, and what this density matrix is—so that it is possible to speak of *the* density matrix of the system. The fact that a system can have two different density matrices at the same time is why we have to focus on the *role* that a density matrix plays for the theoretical treatment of a system, since that is the only way to understand how more than one density matrix can be relevant to the same system.

## 2 Bohmian Mechanics

We begin by briefly recalling Bohmian mechanics. It is a theory of point particles moving in physical space $\mathbb{R}^3$. For the sake of concreteness, consider a universe of $N$ nonrelativistic particles whose positions we denote by $\boldsymbol{Q}_1(t), \ldots, \boldsymbol{Q}_N(t)$. They move according to Bohm's equation of motion,

$$\frac{d\boldsymbol{Q}_j}{dt} = \frac{\hbar}{m_j}\mathrm{Im}\frac{\psi^*\nabla_j\psi}{\psi^*\psi}(\boldsymbol{Q}_1,\ldots,\boldsymbol{Q}_N) \tag{1}$$

where $m_j$ is the mass of particle $j$, $\psi : \mathbb{R}^{3N} \to \mathbb{C}^k$ is the wave function, and $\psi^*\psi$ denotes the scalar product in $\mathbb{C}^k$. In the case $k = 1$ (spin 0), (1) simplifies to

$$\frac{d\boldsymbol{Q}_j}{dt} = \frac{\hbar}{m_j}\mathrm{Im}\frac{\nabla_j\psi}{\psi}(\boldsymbol{Q}_1,\ldots,\boldsymbol{Q}_N)\,. \tag{2}$$

$\psi$ evolves according to the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\sum_{j=1}^{N}\frac{\hbar^2}{2m_j}\Delta_j\psi + V\psi =: \hat{H}\psi \tag{3}$$

where the potential $V$ may take values in the $k\times k$ Hermitian matrices. The configuration $Q(t) = (\boldsymbol{Q}_1(t),\ldots,\boldsymbol{Q}_N(t))$ is random and $|\psi(t)|^2$-distributed at every time $t$,

$$\mathrm{Prob}(Q(t)\in dq) = |\psi(q,t)|^2 dq\,. \tag{4}$$

This is possible because of an equivariance property of (1) and (3): if (4) holds at $t = 0$ then it also holds at every other time. This follows from the following continuity equation, a consequence of (3):

$$\frac{\partial|\psi|^2}{\partial t} = -\,\mathrm{div}\,(|\psi|^2 v) \tag{5}$$

where $v$ is the velocity field, i.e., the (time-dependent) vector field on $\mathbb{R}^{3N}$ whose $j$-th component is the right hand side of (1). We remark that the state at time $t$ of a Bohmian universe is described by the pair $(Q(t),\psi(t))$.

What we describe in this paper about conditional density matrices applies not only to conventional nonrelativistic Bohmian mechanics as just described, but also to Bohmian mechanics on curved manifolds [16, 9], to Bohm's trajectories for Dirac wave functions (see [6, p. 272] and [8]), to the photon trajectories of [17], to the jump processes of [12], and, in a sense that we will explain more fully in Section 7.4, also to theories with a variable number of particles [10, 1, 11, 12].

# 3 Three Density Matrices

If $\mathcal{H}$ denotes the Hilbert space of a system $S$, a density matrix for $S$ is a positive, (bounded) self-adjoint operator $\hat{W} : \mathcal{H} \to \mathcal{H}$ with $\mathrm{tr}\,\hat{W} = 1$. If, as in Bohmian mechanics, $\mathcal{H}$ is a space of wave functions on a configuration space $\mathcal{Q}$, $\mathcal{H} = L^2(\mathcal{Q},\mathbb{C}^k)$, then a density matrix can also be viewed as a function $W : \mathcal{Q}\times\mathcal{Q} \to \mathrm{End}(\mathbb{C}^k)$ (where $\mathrm{End}(\mathbb{C}^k)$

denotes the space of linear mappings (endomorphisms) $\mathbb{C}^k \to \mathbb{C}^k$). The translating relations between the two views, operator on $\mathcal{H}$ and function on $\mathcal{Q} \times \mathcal{Q}$, are

$$\big(\hat{W}\psi\big)^s(q) = \int\limits_{\mathcal{Q}} dq' \sum_{s'} W^s_{s'}(q,q')\,\psi^{s'}(q') \text{ and} \tag{6a}$$

$$W^s_{s'}(q,q') = \langle q, s|\hat{W}|q', s'\rangle \tag{6b}$$

where $s$ and $s'$ index the standard basis of $\mathbb{C}^k$. The function $W$ has the properties

$$W(q',q) = W^*(q,q') \tag{7a}$$

$$0 \leq \int\limits_{\mathcal{Q}} dq \int\limits_{\mathcal{Q}} dq' \sum_{s,s'} \psi^*_s(q)\, W^s_{s'}(q,q')\,\psi^{s'}(q') < \infty \quad \forall \psi \in \mathcal{H} \tag{7b}$$

$$\int\limits_{\mathcal{Q}} dq\, \mathrm{tr}_{\mathbb{C}^k}\, W(q,q) = 1, \tag{7c}$$

where $W^*$ denotes the adjoint endomorphism in $\mathbb{C}^k$, whose matrix is the conjugate transposed. Conversely, the properties (7) are sufficient for $W$ to define a density matrix $\hat{W}$. A particular consequence of (7a) is that on the diagonal of $\mathcal{Q} \times \mathcal{Q}$, $W(q,q)$ is a Hermitian endomorphism (and thus $\mathrm{tr}_{\mathbb{C}^k}\, W(q,q) \in \mathbb{R}$), and a particular consequence of (7b) is that

$$\mathrm{tr}_{\mathbb{C}^k}\, W(q,q) \geq 0 \quad \forall q \in \mathcal{Q}. \tag{8}$$

There are four ways in which density matrices can arise from Bohmian or quantum mechanics. Three of them are well known; we briefly recall them anyway.

1. First, by statistical mixture. Suppose the wave function $\psi$ of a system is random with probability distribution $\mu(d\psi)$ on the unit sphere $\mathscr{S}(\mathcal{H})$ of the Hilbert space $\mathcal{H}$. The associated *statistical density matrix* is

$$\hat{W}_{\mathrm{stat}} = \int\limits_{\mathscr{S}(\mathcal{H})} \mu(d\psi)\, |\psi\rangle\langle\psi| \tag{9a}$$

respectively

$$W_{\mathrm{stat}}{}^s_{s'}(q,q') = \int\limits_{\mathscr{S}(\mathcal{H})} \mu(d\psi)\, \psi^s(q)\, \psi^*_{s'}(q')\,. \tag{9b}$$

This density matrix was first considered in [19]. Note that different distributions $\mu$ may lead to the same density matrix. (For example, the density matrix $\frac{1}{k}I$ on the finite-dimensional Hilbert space $\mathbb{C}^k$ arises from the discrete uniform distribution over the vectors of any orthonormal basis in $\mathbb{C}^k$, as well as from the continuous uniform distribution over the unit sphere $\mathscr{S}(\mathbb{C}^k)$.) The significance of $\hat{W}_{\mathrm{stat}}$ lies in the fact that the distribution of the random outcome $Z$ of an experiment performed on the system depends on $\mu$ only trough $\hat{W}_{\text{stat}}$; i.e., different $\mu$'s leading to the same density matrix also lead to the same statistics of outcomes. More precisely, when the experiment "measures the observable" $\hat{A}$, the probability of obtaining an outcome $Z$ in the set $B \subseteq \mathbb{R}$ is

$$\text{Prob}(Z \in B) = \text{tr}\big(\hat{W}_{\text{stat}} \hat{P}_{\hat{A}}(B)\big) \tag{10}$$

where $\hat{P}_{\hat{A}}$ is the projection-valued measure (PVM) on the real line given by the spectral decomposition of the self-adjoint operator $\hat{A}$.[1] This follows by averaging, according to $\mu$, of the probability that the result is in $B$ given that the state vector of the system is $\psi$, which is (in both standard quantum mechanics and Bohmian mechanics) $\langle\psi|\hat{P}_{\hat{A}}(B)|\psi\rangle$. A particular consequence of (10) is that the outcomes of position measurements are distributed according to the density

$$\rho(q) = \text{tr}_{\mathbb{C}^k} W_{\text{stat}}(q, q) \tag{11}$$

on configuration space $\mathcal{Q}$.

From Schrödinger's equation (3) for $\psi$, one obtains an evolution law [18] for $\hat{W}_{\text{stat}}$:

$$i\hbar \frac{\partial \hat{W}_{\text{stat}}}{\partial t} = [\hat{H}, \hat{W}_{\text{stat}}] \tag{12a}$$

respectively

$$i\hbar \frac{\partial W_{\text{stat}}(q, q')}{\partial t} = \hat{H}_q W_{\text{stat}}(q, q') - \hat{H}_{q'} W_{\text{stat}}(q, q') \tag{12b}$$

where $\hat{H}_q$ means that the Hamiltonian $\hat{H}$ acts on the variable $q$, and [ , ] denotes the commutator. We remark that $\hat{W}_{\text{stat}}$ is "pure," i.e., a projection to a 1-dimensional subspace, if and only if $\mu$ is concentrated on that subspace.

2. The second situation in which a density matrix is relevant involves a system $S_1$ that is entangled with another system $S_2$. In this case, the composite system $S_1 \cup S_2$ possesses a wave function $\Psi^{s_1 s_2}(q_1, q_2)$ or $\Psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$, but no wave function is associated with $S_1$ alone. However, the following *reduced density matrix* can be associated with $S_1$:

$$\hat{W}_{\text{red}} = \text{tr}_2 \, |\Psi\rangle\langle\Psi| \tag{13a}$$

[1] We remind the reader that in Bohmian mechanics such an experiment need not *measure* anything in the literal sense of the word [4, 14]. We also note that (10) holds not only for "measurements of observables," but for arbitrary experiments $\mathcal{E}$ with results in the value space $\mathcal{V}$: with every $\mathcal{E}$ is associated a positive-operator-valued measure (POVM) $\hat{P}_{\mathcal{E}}$ [7, 14] such that the probability of obtaining from $\mathcal{E}$ an outcome in the set $B \subseteq \mathcal{V}$ is $\text{tr}\big(\hat{W}_{\text{stat}} \hat{P}_{\mathcal{E}}(B)\big)$.

respectively

$$W_{\mathrm{red}}{}^{s_1}_{s_1'}(q_1, q_1') = \int\limits_{\mathcal{Q}_2} dq_2 \sum_{s_2} \Psi^{s_1 s_2}(q_1, q_2)\, \Psi^*_{s_1' s_2}(q_1', q_2) \tag{13b}$$

where $\mathrm{tr}_2$ denotes the partial trace over $\mathcal{H}_2$. This kind of density matrix was first considered in [15]. Note that $\hat{W}_{\mathrm{red}}$ is an operator on $\mathcal{H}_1$. Like $\hat{W}_{\mathrm{stat}}$, $\hat{W}_{\mathrm{red}}$ possesses significance in terms of probability distributions: if one "measures" $\hat{A}$ on $S_1$ alone, then the probability of obtaining a result $Z$ in the set $B \subseteq \mathbb{R}$ is

$$\mathrm{Prob}(Z \in B) = \mathrm{tr}\big(\hat{W}_{\mathrm{red}} \hat{P}_{\hat{A}}(B)\big) \tag{14}$$

where the trace is, of course, taken in $\mathcal{H}_1$. This equation follows from the fact that the observable on $\mathcal{H}_1 \otimes \mathcal{H}_2$ that corresponds to this experiment, as an experiment on $S_1 \cup S_2$, is $\hat{A} \otimes \hat{1}$, so that the probability for $Z \in B$ is $\langle \Psi | \hat{P}_{\hat{A}}(B) \otimes \hat{1} | \Psi \rangle$, which equals (14).

If $S_1$ and $S_2$ are decoupled, i.e., if $\hat{H} = \hat{H}_1 \otimes \hat{1} + \hat{1} \otimes \hat{H}_2$, the reduced density matrix evolves in the same way as statistical density matrices do, governed by $\hat{H}_1$:

$$i\hbar \frac{\partial \hat{W}_{\mathrm{red}}}{\partial t} = [\hat{H}_1, \hat{W}_{\mathrm{red}}] \tag{15a}$$

respectively

$$i\hbar \frac{\partial W_{\mathrm{red}}(q, q')}{\partial t} = \hat{H}_{1q} W_{\mathrm{red}}(q, q') - \hat{H}_{1q'} W_{\mathrm{red}}(q, q')\,. \tag{15b}$$

In case $S_1$ and $S_2$ are coupled, $W_{\mathrm{red}}$ does not have an autonomous dynamics, i.e., its evolution depends on the $\Psi$ from which it arises. We remark that $\hat{W}_{\mathrm{red}}$ is "pure" if and only if $S_1$ and $S_2$ are disentangled, $\Psi^{s_1 s_2}(q_1, q_2) = \psi_1^{s_1}(q_1)\, \psi_2^{s_2}(q_2)$.

3. The third possibility is the combination of the first and the second types of density matrices: the reduced density matrix of a statistical mixture. Suppose the wave function $\Psi$ of the system $S_1 \cup S_2$ is random with distribution $\mu$ on $\mathscr{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$. Then define the *combined density matrix* by

$$\hat{W}_{\mathrm{comb}} = \int\limits_{\mathscr{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)} \mu(d\Psi)\, \mathrm{tr}_2\, |\Psi\rangle\langle\Psi| \tag{16a}$$

respectively

$$W_{\mathrm{comb}}{}^{s_1}_{s_1'}(q_1, q_1') = \int\limits_{\mathscr{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)} \mu(d\Psi) \int\limits_{\mathcal{Q}_2} dq_2 \sum_{s_2} \Psi^{s_1 s_2}(q_1, q_2)\, \Psi^*_{s_1' s_2}(q_1', q_2)\,. \tag{16b}$$

This kind of density matrix was first considered in [18, p. 424]. $\hat{W}_{\text{comb}}$ can be obtained either by averaging the reduced density matrix associated with the random state $\Psi$, or by reducing, i.e., taking the partial trace of, the statistical density matrix on $\mathcal{H}_1 \otimes \mathcal{H}_2$ associated with $\mu$. Again, the probability that the result $Z$ of an experiment on $S_1$ "measuring" $\hat{A}$ lies in the set $B \subseteq \mathbb{R}$ is

$$\text{Prob}(Z \in B) = \text{tr}\big(\hat{W}_{\text{comb}} \hat{P}_{\hat{A}}(B)\big)\,. \tag{17}$$

This follows either from averaging (14) over $\mu$ or from applying (10) to $\hat{A} \otimes \hat{1}$.

Like the reduced density matrix, $\hat{W}_{\text{comb}}$ follows the unitary evolution governed by $\hat{H}_1$ whenever that makes sense, i.e., whenever $S_1$ and $S_2$ are decoupled. $\hat{W}_{\text{comb}}$ is pure if and only if $\mu$ is concentrated on the subspace $\mathbb{C}\psi_1 \otimes \mathcal{H}_2$ for some $\psi_1 \in \mathcal{H}_1$.

# 4 A Fourth Density Matrix

We now turn to the fourth, novel, kind of density matrix: the conditional density matrix. It also involves a system $S_1$ that is entangled with $S_2$, and it is related to the notion of conditional wave function [13] which we recall first. For the sake of definiteness, we take $S_2$ to be the environment of $S_1$, i.e., the rest of the universe.

In Bohmian mechanics for spin 0 particles, more precisely in Bohmian mechanics with complex-valued wave functions, the *conditional wave function* of $S_1$ is obtained from the wave function $\Psi(q_1, q_2)$ of $S_1 \cup S_2$ by inserting the actual configuration $Q_2$ of $S_2$,

$$\psi_{\text{cond}}(q_1) = \frac{1}{\sqrt{\mathcal{N}}}\Psi(q_1, Q_2) \tag{18a}$$

$$\text{where } \mathcal{N} = \int\limits_{\mathcal{Q}_1} dq_1\, |\Psi(q_1, Q_2)|^2 \tag{18b}$$

is a normalizing factor ensuring that $\int |\psi_{\text{cond}}|^2 = 1$. $\psi_{\text{cond}}$ can be viewed as the wave function of $S_1$ alone. It does not, in general, evolve according to a Schrödinger equation (3), indeed it does not have an autonomous dynamics at all.[2] In fact, in appropriate situations the evolution of $\psi_{\text{cond}}$ leads to collapse, in the usual textbook manner, which seems quite appropriate for the wave function of a subsystem. $\psi_{\text{cond}}$ shares the following basic properties with the wave function $\psi$ in Bohmian mechanics:

- The conditional distribution of $Q_1$ given $Q_2$ is $|\psi_{\text{cond}}|^2$. More precisely, we have the following formula for the conditional probability:

$$\text{Prob}(Q_1 \in dq_1 | Q_2) = |\psi_{\text{cond}}(q_1)|^2 dq_1\,, \tag{19}$$

[2]The conditional wave function at time $t = 0$ need not determine the conditional wave function at later times. As an example, consider two situations with the same $\Psi$, the same $Q_2(0)$ and different $Q_1(0)$: since $\psi_{\text{cond}}$ does not depend on $Q_1$, it will be the same in the two situations at $t = 0$, but since the motion of $Q_2$ typically depends on $Q_1$, the two situations will typically have different $Q_2$'s at later times, and thus typically different $\psi_{\text{cond}}$'s.

which resembles the formula (4) for the probability in terms of the wave function. (19) follows from the fact that the pair $(Q_1, Q_2)$ is $|\Psi|^2$ distributed.

- The motion of $Q_1$ can be computed from $\psi_{\mathrm{cond}}$ according to

$$\frac{d\boldsymbol{Q}_{1j}}{dt} = \frac{\hbar}{m_{1j}} \mathrm{Im} \frac{\nabla_{1j}\psi_{\mathrm{cond}}}{\psi_{\mathrm{cond}}}(\boldsymbol{Q}_{11}, \ldots, \boldsymbol{Q}_{1N_1}), \tag{20}$$

which is the same formula as (2) for the velocity in terms of the wave function.

An analogous conditional wave function cannot be formed, however, when the particles of $S_2$ have spin or any other internal degree of freedom entailing that the wave function has several complex components. The reason is that $\psi_{\mathrm{cond}}$ as defined in (18a) would have too many components, i.e., more spin indices than appropriate for a wave function of $S_1$ alone. In particular, $\psi_{\mathrm{cond}}$ would not be an element of $\mathcal{H}_1$.

We propose to consider instead the *conditional density matrix*, which is obtained from $\Psi(q_1, q_2)\,\Psi^*(q_1', q_2')$ by inserting the actual configuration $Q_2$ of $S_2$ for both $q_2$ and $q_2'$, and contracting over the spin index belonging to $S_2$:

$$W_{\mathrm{cond}}{}^{s_1}_{s_1'}(q_1, q_1') = \frac{1}{\mathcal{N}} \sum_{s_2} \Psi^{s_1 s_2}(q_1, Q_2)\, \Psi^*_{s_1' s_2}(q_1', Q_2) \tag{21}$$

with normalizing factor[3]

$$\mathcal{N} = \int_{\mathcal{Q}_1} dq_1 \sum_{s_1 s_2} \Psi^{s_1 s_2}(q_1, Q_2)\, \Psi^*_{s_1 s_2}(q_1, Q_2)\,. \tag{22}$$

One easily checks that $W_{\mathrm{cond}}$ satisfies (7) and thus is a density matrix.[4] The expression for the corresponding operator $\hat{W}_{\mathrm{cond}}$ reads

$$\hat{W}_{\mathrm{cond}} = \frac{\mathrm{tr}_2\big(|\Psi\rangle\langle\Psi|\hat{1}\otimes \hat{P}_{\hat{q}_2}(dq_2)\big)}{\mathrm{tr}\big(|\Psi\rangle\langle\Psi|\hat{1}\otimes \hat{P}_{\hat{q}_2}(dq_2)\big)}(q_2 = Q_2) \tag{23}$$

where $\hat{P}_{\hat{q}_2}$ is the projection-valued measure on $\mathcal{Q}_2$ defined by the joint spectral decomposition of all position operators of $S_2$, and the fraction is a Radon–Nikodým derivative of an operator-valued measure on $\mathcal{Q}_2$ with respect to a real-valued measure on $\mathcal{Q}_2$, and thus an operator-valued function on $\mathcal{Q}_2$, into which we insert $Q_2$.

We remark that $\hat{W}_{\mathrm{cond}}$ is pure if and only if $\Psi(q_1, Q_2)$ as an element of $L^2(\mathcal{Q}_1, \mathbb{C}^{k_1}) \otimes \mathbb{C}^{k_2}$ is a tensor product, $\Psi^{s_1 s_2}(q_1, Q_2) = \psi_1^{s_1}(q_1)\,\psi_2^{s_2}$. In particular, $\hat{W}_{\mathrm{cond}}$ is pure if $\Psi$ is complex valued.

The conditional density matrix has the following properties analogous to those of the conditional wave function:

[3] One can show that for almost every configuration $Q = (Q_1, Q_2)$ (almost every with respect to the $|\Psi|^2$ distribution), $\mathcal{N}$ will be neither zero nor infinite.

[4] The only step that may not be obvious is the finiteness part of (7b), which follows from the fact that $\mathcal{N} < \infty$ so that for any fixed value of $s_2$, $\Psi^{s_1 s_2}(q_1, Q_2)$ as a function of $s_1$ and $q_1$ lies in $L^2(\mathcal{Q}_1, \mathbb{C}^{k_1})$; thus the scalar product with any $\psi \in L^2(\mathcal{Q}_1, \mathbb{C}^{k_1})$ is finite.

- The conditional distribution of $Q_1$ given $Q_2$ can be computed from $W_{\mathrm{cond}}$ by taking the trace on the diagonal. More precisely, we have the following formula for the conditional probability:

$$\mathrm{Prob}(Q_1 \in dq_1 | Q_2) = \mathrm{tr}_{\mathbb{C}^{k_1}} W_{\mathrm{cond}}(q_1, q_1)\, dq_1 \,. \tag{24}$$

  This follows from the fact that the pair $(Q_1, Q_2)$ is $|\Psi|^2$ distributed. Note that the right hand side is the usual expression (11) for the probability distribution on configuration space when a system is described by a density matrix.

- The motion of $Q_1$ can be computed from $W_{\mathrm{cond}}$ according to

$$\frac{d\boldsymbol{Q}_{1j}}{dt} = \frac{\hbar}{m_{1j}} \mathrm{Im} \frac{\nabla_{\boldsymbol{q}_{1j}} \mathrm{tr}_{\mathbb{C}^{k_1}} W_{\mathrm{cond}}(q_1, q_1')}{\mathrm{tr}_{\mathbb{C}^{k_1}} W_{\mathrm{cond}}(q_1, q_1')} (q_1 = q_1' = Q_1) \,. \tag{25}$$

To be able to appreciate (25), we have to consider a fifth type of density matrix.

# 5 A Fifth Density Matrix

A density matrix is relevant in yet another way: in a modified version of Bohmian mechanics in which the particles are guided not by a wave function but by a density matrix. Let us call this $W$-Bohmian mechanics. Whereas in the conventional version of Bohmian mechanics the wave function (of the universe) is something real, as an objective component of the state of the universe at a given time, in $W$-Bohmian mechanics instead of a wave function (of the universe) we may have only a density matrix. This density matrix does not arise in any way from an analysis of the theory, but is built into the fundamental postulates of $W$-Bohmian mechanics. It is a *fundamental density matrix*, $W_{\mathrm{fund}}$, in contrast to the four other density matrices we have discussed, which were derived objects, derived from $\psi$ and $Q$. Like the conditional density matrix, $W_{\mathrm{fund}}$ has not been considered previously in the literature. The state at time $t$ of a $W$-Bohmian universe is given by the pair $(Q(t), W_{\mathrm{fund}}(t))$, and it evolves according to

$$\frac{d\boldsymbol{Q}_j}{dt} = \frac{\hbar}{m_j} \mathrm{Im} \frac{\nabla_{\boldsymbol{q}_j} \mathrm{tr}_{\mathbb{C}^k} W_{\mathrm{fund}}(q, q')}{\mathrm{tr}_{\mathbb{C}^k} W_{\mathrm{fund}}(q, q')} (q = q' = Q) \tag{26}$$

as the equation of motion for $Q$, and

$$i\hbar \frac{\partial \hat{W}_{\mathrm{fund}}}{\partial t} = [\hat{H}, \hat{W}_{\mathrm{fund}}] \tag{27a}$$

respectively

$$i\hbar \frac{\partial W_{\mathrm{fund}}(q, q')}{\partial t} = \hat{H}_q W_{\mathrm{fund}}(q, q') - \hat{H}_{q'} W_{\mathrm{fund}}(q, q') \tag{27b}$$

for $\hat{W}_{\rm fund}$, respectively $W_{\rm fund}(q,q')$. Note that equations (27) are the same as (12) and (15). (26) was first written down by Bell [2] for the purpose of contrasting it with the implications of Bohm's equation of motion (1) for a system with a random wave function, hence described by $\hat{W}_{\rm stat}$.

The configuration $Q(t)$ is random with distribution given by the trace of the diagonal of $W_{\rm fund}(t)$, i.e.,

$$\mathrm{Prob}(Q(t) \in dq) = \mathrm{tr}_{\mathbb{C}^k}\, W_{\rm fund}(q,q,t)\, dq. \tag{28}$$

This is possible because of the following equivariance theorem: if (28) holds at $t=0$ then it also holds at every other time. To see this, note that (27) implies that

$$\frac{\partial \mathrm{tr}_{\mathbb{C}^k}\, W_{\rm fund}(q,q)}{\partial t} = -\,\mathrm{div}\left(\mathrm{tr}_{\mathbb{C}^k}\, W_{\rm fund}(q,q)\, v\right) \tag{29}$$

where $v$ is the velocity field, i.e., the (time-dependent) vector field on $\mathcal{Q}$ whose $j$-th component is the right hand side of (26).

# 6 Discussion

Bohmian mechanics, as described in Section 2, is a special case of $W$-Bohmian mechanics: if $W_{\rm fund}$ is pure, i.e., if it arises from a wave function $\psi$ via

$$W_{{\rm fund}\,s'}^{\;s}(q,q') = \psi^s(q)\, \psi^*_{s'}(q')\,, \tag{30}$$

then the equation of motion (26) reduces to Bohm's equation of motion (1), the probability law (28) reduces to the $|\psi|^2$ law (4), and the evolution (27) entails that $W_{\rm fund}$ remains pure and arises from a wave function that evolves according to the Schrödinger equation (3).

Conversely, the equations (26) and (28) of $W$-Bohmian mechanics arise for the behavior of subsystems from Bohmian mechanics for systems of many particles with spin: The motion of the particles of subsystem $S_1$ is governed according to (25) by a density matrix, $\hat{W}_{\rm cond}$, in the same way as in $W$-Bohmian mechanics the motion of particles is governed according to (26) by a density matrix, $\hat{W}_{\rm fund}$. In addition to the velocities, also the probabilities (24) are determined by a density matrix in the same way as in $W$-Bohmian mechanics (28). Thus, even were the universe as a whole governed by Bohmian mechanics, for most subsystems the state would be described by a density matrix, $W_{\rm cond}$, with the velocities and probabilities of the subsystem governed by the equations of $W$-Bohmian mechanics for $W_{\rm cond}$. In this sense, $W$-Bohmian mechanics is the theory relevant to most systems in a Bohmian universe. (More precisely, this holds for all those systems for which $\hat{W}_{\rm cond}$ is not pure.)

A big difference, however, between the dynamics of a subsystem and $W$-Bohmian mechanics lies in the fact that, unlike the fundamental density matrix, see (27), the conditional density matrix need not evolve unitarily. Nevertheless, there are special situations in which $W_{\rm cond}$ does evolve unitarily, at least as a good approximation. This happens trivially when $S_1$ and $S_2$ are disentangled, $\Psi(q_1,q_2) = \psi_1(q_1) \otimes \psi_2(q_2)$, and decoupled (so that they stay disentangled). It also happens when (and for as long as) $S_1$ and $S_2$ are decoupled and

$$\Psi(q_1, q_2) = \psi_1(q_1) \otimes \psi_2(q_2) + \Psi^{\perp}(q_1, q_2), \tag{31}$$

i.e.,

$$\Psi^{s_1 s_2}(q_1, q_2) = \psi_1^{s_1}(q_1)\, \psi_2^{s_2}(q_2) + (\Psi^{\perp})^{s_1 s_2}(q_1, q_2), \tag{32}$$

where $\psi_2$ and $\Psi^{\perp}$ have disjoint $q_2$-supports and $Q_2 \in \text{support}\, \psi_2$. Such a situation often occurs after a measurement, and indeed allows us to regard $\psi_1$ as the (effective) wave function of $S_1$, obeying Schrödinger's equation (3). For spin 0, (32) characterizes the situation in which we can expect the conditional wave function to evolve unitarily; thus, the conditional density matrix evolves unitarily in all situations in which the conditional wave function would for spin 0. We obtain another case of unitarily evolving $W_{\text{cond}}$ by replacing (32) by

$$\Psi^{s_1 s_2}(q_1, q_2) = \psi_1^{s_1 s_2}(q_1)\, \psi_2(q_2) + (\Psi^{\perp})^{s_1 s_2}(q_1, q_2), \tag{33}$$

with a complex-valued $\psi_2$, and assuming in addition that the Hamiltonian $\hat{H}_2$ for $S_2$ involves no interaction between spin and configurational degrees of freedom.

For example, consider an EPR–Bohm–Bell pair of spin 1/2 particles, each headed towards its Stern–Gerlach magnet, with $q_1$ and $q_2$ the positions of the particles. Suppose both magnets are oriented so as to measure $\sigma_z$ and that the geometry is such that particle 1 completely passes its SG magnet before particle 2 reaches its SG magnet. Initially the spin state is the singlet state, depending on neither $q_1$ nor $q_2$, and we may assume as well that the configuration space wave packet is initially of product form $\psi_1(q_1)\psi_2(q_2)$. Then the initial wave function is of the form (33) with $\Psi^{\perp} = 0$ and (regarding the possible values of $s_i$ as $\pm 1$)

$$\psi_1^{s_1 s_2}(q_1) = \frac{1}{\sqrt{2}}(\delta_{s_1,1}\delta_{s_2,-1} - \delta_{s_1,-1}\delta_{s_2,1})\psi_1(q_1)\,, \tag{34}$$

corresponding to

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right) \otimes \psi_1 \tag{35}$$

in the standard $\sigma_z$ representation.

Until particle 1 reaches its magnet the Schrödinger evolution preserves this form and $\hat{W}_{\text{cond}} = \frac{1}{2} I \otimes |\psi_1\rangle\langle\psi_1|$, where $\psi_1 = \psi_1(t)$ obeys Schrödinger's equation for particle 1. Moreover, until particles 2 reaches its magnet (i.e., in the absence of a magnetic field acting on particle 2), $\hat{H}_2$ involves no coupling between spin and translational degrees of freedom, so that the form (33) is preserved and $\hat{W}_{\text{cond}}$ evolves unitarily according to (27), even after particle 1 has reached its magnet. After particle 1 has passed trough its magnet (but before particle 2 reaches its magnet) $\hat{W}_{\text{cond}} = \frac{1}{2}(\hat{W}_{\text{up}} + \hat{W}_{\text{down}})$, where $\hat{W}_{\text{up}}$, respectively $\hat{W}_{\text{down}}$, corresponds to the pure state $|\uparrow\rangle \otimes \psi_{\text{up}}$, respectively $|\downarrow\rangle \otimes \psi_{\text{down}}$, the states to which $|\uparrow\rangle \otimes \psi_1$, respectively $|\downarrow\rangle \otimes \psi_1$, would evolve under the Schrödinger evolution for particle 1. After particle 2 reaches its magnet, $\hat{W}_{\text{cond}}$ no longer evolves unitarily (or even autonomously). Rather it collapses either to $\hat{W}_{\text{up}}$ or $\hat{W}_{\text{down}}$ according to whether the initial configuration is such that $Q_2$ ends up going down or up.

Throughout the course of the entire experiment $Q_1$ evolves according to (25). (Note also that after particle 2 has crossed its magnet, (33) is again approximately satisfied, with $\Psi^{\perp}$ the wave packet that does not contain $Q_2$.)

We now turn to the relations between the various density matrices, and discuss first the relation between $W_{\text{cond}}$ and $W_{\text{red}}$. $W_{\text{red}}$ is the average conditional density matrix, with the average taken with respect to quantum equilibrium, i.e., over the ensemble in which $Q = (Q_1, Q_2)$ is $|\Psi|^2$ distributed:

$$W_{\text{red}}{}^{s_1}_{s_1'}(q_1, q_1') = \int\limits_{\mathcal{Q}_1 \times \mathcal{Q}_2} dQ_1\, dQ_2\, |\Psi(Q_1, Q_2)|^2\, W_{\text{cond}}{}^{s_1}_{s_1'}(q_1, q_1')(Q_2). \tag{36}$$

This relation makes clear that a system can have a conditional and a reduced density matrix at the same time, the two being different from each other: the conditional density matrix of a system depends on the configuration $Q_2$ of its environment; when this dependence is averaged out by taking the quantum equilibrium expected value one obtains the reduced density matrix of the system. (Note that for spin 0 (36) is the quantum equilibrium average of $|\psi_{\text{cond}}\rangle\langle\psi_{\text{cond}}|$.)

Similarly, the combined (reduced statistical) density matrix is an average of the conditional density matrix, with the average taken over the ensemble in which $\Psi$ is $\mu$ distributed and, given $\Psi$, $Q$ is $|\Psi|^2$ distributed:

$$W_{\text{comb}}{}^{s_1}_{s_1'}(q_1, q_1') = \int\limits_{\mathscr{S}(\mathcal{H})} \mu(d\Psi) \int\limits_{\mathcal{Q}_1 \times \mathcal{Q}_2} dQ_1\, dQ_2\, |\Psi(Q_1, Q_2)|^2\, W_{\text{cond}}{}^{s_1}_{s_1'}(q_1, q_1')(Q_2, \Psi). \tag{37}$$

Of course, $W_{\text{stat}}$ can also be viewed as an average (of $|\psi\rangle\langle\psi|$) over the ensemble with $\mu$-distributed $\psi$, but this does not involve the conditional density matrix.

The fact that $W_{\text{cond}}$ determines the Bohmian velocities according to (25) should be contrasted with the failure of such a connection for $W_{\text{stat}}$, $W_{\text{red}}$, and $W_{\text{comb}}$: If the wave function $\psi$ of a system is random, the Bohmian velocities have to be computed from the actual realization of $\psi$, and thus could assume different values, corresponding to different $\psi$'s, even when $Q$ is held fixed. Inserting, for example, $W_{\text{stat}}$ in a formula like (25) or (26) would yield, in contrast, an average velocity at $Q$, averaged over the ensemble of different $\psi$'s (with the additional $Q$-dependent weight proportional to $|\psi(Q)|^2$). This is what Bell referred to in the phrase we quoted in the beginning, and what he elucidated in [2]. Similarly, since $W_{\text{red}}$ is the average of the conditional density matrix, over a certain ensemble, it leads to an average velocity (in fact to the best guess at the velocity that one could make without knowing $Q_2$). In contrast, $W_{\text{cond}}$ depends on the actual value of $Q_2$ and yields the true Bohmian velocity, as defined by (1) and the wave function of the universe.

The statistical analysis of Bohmian mechanics in [13] remains valid when conditional wave functions are replaced by conditional density matrices.

# 7 Remarks

## 7.1 Conditional Density Matrix in Orthodox Quantum Mechanics

In orthodox quantum mechanics, the definition (21) of the conditional density matrix cannot be written down, for lack of a configuration $Q_2$ that could be inserted into $\Psi$. However, orthodox quantum mechanics arguably maintains that macroscopic objects can be viewed and treated classically, which presumably means that there should exist something like a "macroscopic configuration." In case that $\Psi$ is such that the conditional density matrix does not change much with the microscopic details of $Q_2$ (i.e., that it is quite accurately determined by merely the macroscopic information about $Q_2$), a conditional density matrix also makes sense in orthodox quantum mechanics. In this case the conditional density matrix of orthodox quantum mechanics would equal, within its accuracy, the one of Bohmian mechanics. Another way of obtaining this density matrix is to collapse the wave function (to the region of configuration space having $q_2$ compatible with the actual macroscopic configuration of $S_2$), and then to take the reduced density matrix.

## 7.2 Second Quantization

In [12], we describe a construction that might be called the "second quantization of a Markov process." Parallel to the "second quantization" algorithm of forming a Fock space out of a given 1-particle Hilbert space and the free Hamiltonian on Fock space out of a given 1-particle Hamiltonian, this construction builds a dynamics on the configuration space of a variable number of particles out of a given 1-particle dynamics. A key step in this construction is a general procedure for forming the law of motion for $N$ particles, given an *arbitrary* 1-particle law. Interestingly, the conditional density matrix is indispensable for this procedure (except when wave functions are complex–valued).

A Bohm-type law of motion for one particle associates a velocity vector field on $\mathbb{R}^3$ with every (smooth) 1-particle wave function. We now regard this association abstractly as a given mapping, from which we want to systematically construct the $N$-particle law that provides the velocities of all particles from an $N$-particle wave function and the positions of all particles. By inserting the positions of all but one particle into the wave function, we get a conditional object for one particle—for spin 0 a conditional wave function, otherwise a conditional density matrix. Only if the one-particle law associates with this conditional object a velocity vector field on $\mathbb{R}^3$, can we insert the position of the remaining particle into the vector field and get the particle's velocity. For spin $> 0$ we thus need more than what we mentioned at the beginning of this paragraph: we need that the one-particle law provide a velocity field *for every density matrix*, as $W$-Bohmian mechanics does, and not merely for every wave function.

## 7.3 Empirical Consequences of $W$-Bohmian Mechanics

One may wonder whether one can decide empirically between Bohmian mechanics and $W$-Bohmian mechanics, or, in other words, whether one can determine empirically in a universe governed by $W$-Bohmian mechanics if the fundamental density matrix is pure (30). The question is delicate. We think that the answer is no, for the following reason: compare a $W$-Bohmian universe with a Bohmian universe with a random wave function such that the associated statistical density matrix equals the fundamental density matrix of the $W$-Bohmian universe. Since an empirical decision, if it can be made at time $t_0$, would have to be based solely on the configuration $Q_{t_0}$ at that time, and since the distribution of $Q_{t_0}$ is the same in both situations, it seems that there cannot be a detectable difference: A given $Q_{t_0}$ could as well have arisen from an appropriate wave function from the random wave function ensemble as from the corresponding fundamental density matrix.

What makes the question delicate, however, is, in part, the following: we might not take seriously a theory involving a wave function of the universe or a density matrix of the universe that is "unreasonable" or "conspiratorial." Therefore, the question is connected to questions such as what would count as a "reasonable" $W_{\text{fund}}$, and whether a statistical mixture mimicking a given "reasonable" $W_{\text{fund}}$ might have to contain some "unreasonable" wave functions.

## 7.4 Conditioning on Spatial Regions

It is often desirable to define the subsystems $S_i$, $i = 1, 2$, as encompassing all those particles which are presently located in the regions $R_i \subseteq \mathbb{R}^3$, with $R_1 \cup R_2 = \mathbb{R}^3$ and $R_1 \cap R_2 = \emptyset$. To condition on the configuration $Q_2$ of $S_2$ then means to condition on the configuration in the region $R_2$. We describe below what appears to be the most convenient way to carry out such a conditioning on a spatial region. One might suspect that conditioning on a spatial region is a very complicated story. But, in fact, it could not be simpler.

Since the number of particles in the region $R_i$ can vary over time, it is helpful to consider right from the start a configuration space of a variable number of particles. We consider the space

$$\Gamma(\mathbb{R}^3) := \bigcup_{n=0}^{\infty} \mathbb{R}^{3n}/S_n \tag{38}$$

where $S_n$ denotes the group of permutations of $n$ objects, which acts on $\mathbb{R}^{3n}$ by permuting the particle labels. A configuration from $\Gamma(\mathbb{R}^3)$ represents any number of identical (unlabeled) particles. For a discussion of this space, see [12].

We can extend the definition of $\Gamma$ to arbitrary sets $R$,

$$\Gamma(R) := \bigcup_{n=0}^{\infty} R^n/S_n. \tag{39}$$

When $R \subset \mathbb{R}^3$, $\Gamma(R)$ can be viewed as a subset of $\Gamma(\mathbb{R}^3)$, containing those configurations for which all particles are located in $R$. Now observe that, when $R_1$ and $R_2$ are disjoint sets, then

$$\Gamma(R_1 \cup R_2) = \Gamma(R_1) \times \Gamma(R_2)\,. \tag{40}$$

This property is helpful, as it tells us that the definition of the subsystems $S_i$ in terms of spatial regions $R_i$ leads to a Cartesian product decomposition $\mathcal{Q} = \mathcal{Q}_1 \times \mathcal{Q}_2$ of configuration space, and thus allows us to use, without change, all of our considerations on conditional density matrices, which assumed such a decomposition.

# 8 Conclusions

We have introduced the notion of conditional density matrix in Bohmian mechanics, and contrasted it, on the one hand, with the notion of conditional wave function, and on the other hand, with various other notions of density matrices. In contrast to the statistical, reduced, or combined (reduced statistical) density matrix, the conditional density matrix possesses direct significance for the particle velocities.

The fact that with the same system can be associated several density matrices brings into sharp focus that the *meaning* of a density matrix is not a priori; instead, various meanings are conceivable. Ultimately, the meaning of a density matrix arises from its relevance to the primitive objects, such as particle world lines, that the theory is about. In Bohmian mechanics, the various types of density matrices that we have considered are all relevant to the particles, but in very different ways.

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