

MEANING OF THE DENSITY MATRIX

Y. Aharonov*[†] and J. Anandan*

*Department of Physics and Astronomy

University of South Carolina

Columbia SC 29208, USA

E-mail: jeeva@sc.edu

and

[†] School of Physics, Tel Aviv University

Ramat Aviv, Tel Aviv, Israel

Abstract

Protective measurement, which was proposed as a method of observing the wavefunction of a single system, is extended to the observation of the density matrix of a single system. d’Espagnat’s definition of ‘proper mixture’ is shown to be improper because it does not allow for appropriate fluctuations. His claim that there could be different mixtures corresponding to the same density matrix is critically examined. These results provide a new meaning to the density matrix, which gives it the same ontological status as the wavefunction describing a pure state. This also enables quantum entropy to be associated with a single system.

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1 Introduction

It is well known that quantum mechanics may be formulated by specifying the state of a quantum system by either a statevector that belongs to the Hilbert space or by a ‘density matrix’ that is a Hermitian operator ρ acting on the Hilbert space with non negative eigenvalues whose sum is 1. The density matrix has the advantage that not only does it describe a pure state that satisfies the condition $\rho^2 = \rho$, which can equally well be described by a state vector, but also it can describe a mixed state which cannot be described by a state vector.

The traditional meaning given to the density matrix is that its eigenvalues are the probabilities for finding the system in the corresponding eigenstates. The only way we know of giving physical meaning to the probabilities of outcomes is by interpreting them as relative frequencies of the corresponding states in an appropriate ensemble of N identical copies of the system that are in the various possible states and taking the limit of $N \rightarrow \infty$.

But there are three drawbacks to this meaning due to the fact that the ensemble associated with ρ by this prescription is not unique: (1) When two or more eigenvalues of ρ are equal, the basis of eigenstates of ρ is not unique. (2) If a usual measurement is made of an observable A that does not commute with ρ , then the possible outcomes, which are eigenstates of A , are in general different from the eigenstates of ρ . Hence ρ undergoes a sudden change to a new density matrix ρ' whose eigenstates are the eigenstates of A . This is the quantum measurement problem stated more generally than the usual statement in which ρ represents a pure state. Even if this discontinuity in evolution is accepted, unless the eigenvalues of A are all distinct, the ensemble associated with ρ' , according to the above prescription, is not unique. (3) As we shall see later, the interpretation of the probabilities as relative frequencies is not possible for a fixed finite N . We also cannot set $N = \infty$ because then the relative frequencies would be ratios of infinities which are not mathematically meaningful. So, it is necessary to take the limit of $N \rightarrow \infty$. We then need to associate with ρ a

sequence of finite ensembles with ever increasing N , with none of the members of the sequence providing a physical meaning to ρ , except in some approximate sense. It appears to us that this sequence is merely a conceptualization and does not provide an objective reality that could be described by the density matrix.

In this paper we provide a new meaning to the density matrix which does not have the above drawbacks. We shall be concerned, in this investigation, with the following questions: (A) Does the density matrix of a system uniquely determine the state of the system? (B) Can the density matrix be associated with a single system, as opposed to an ensemble? We shall answer both these questions affirmatively, and in the process correct some common misconceptions concerning the density matrix. The new meaning we shall give to the density matrix will be based primarily on generalizing a method for observing a pure state by means of ‘protective measurements’ on a *single* system in that state[2] to the observation of the density matrix of a *single* system. The philosophical aspects of this work will be discussed elsewhere[1].

2 Protective Measurements of the Density Matrix

To fix our ideas, we shall consider just one way of doing protective measurements: The state of the quantum system under observation is in an eigenstate, described by the state vector $|\psi\rangle$, of the Hamiltonian H with non degenerate eigenvalue. An observable A is measured adiabatically in a time interval $T \gg \frac{\hbar}{|\Delta E|}$, where ΔE is the energy difference between the energy of the given state and the nearest energy eigenvalue, so that there is no appreciable change in the state. This results in the observation of $\langle \psi|A|\psi\rangle = \text{tr } \rho A$ although only a single system is being used[2], where $\rho = |\psi\rangle\langle\psi|$ is the density matrix of this pure state. By doing protective observations of sufficient number of observables A the state vector $|\psi\rangle$ may be determined up to phase. Since the

phase is undetermined, protective measurements really determine the system's density matrix ρ and not its state vector.

In the above procedure it was assumed that the system was in a non entangled state prior to the interaction with the apparatus. Then the interaction with the apparatus does not lead to any entanglement. But in an actual experiment, some interaction of the system with the environment is unavoidable. So, let us consider the system under consideration and another system in an entangled state. Then without loss of generality the state of the combined system may be written as

$$|\chi\rangle = \sum_i c_i |\psi_i\rangle |\phi_i\rangle \quad (1)$$

where the $|\psi_i\rangle$ and $|\phi_j\rangle$ are, respectively, orthonormal states of the first and the second system.

The protective measurement of a state of two systems, represented by $|\chi\rangle$, has been studied by one of us[3]. If the observable, represented by the Hermitian operator A , that is so measured is that of the first system only, then the result of the protective measurement is

$$\langle \chi | A | \chi \rangle = \sum_i |c_i|^2 \langle \psi_i | A | \psi_i \rangle = \text{tr} \rho A \quad (2)$$

where $\rho = \sum_i |c_i|^2 |\psi_i\rangle \langle \psi_i|$ is the reduced density matrix of the first system. Thus the possible pure states in which the system can be in which are represented by ρ all contribute with the appropriate weights to the result of the protective measurement which is a single number, such as the displacement of the pointer in an apparatus. This is very different from the protective observation of a single pure state which was studied previously[2, 3]. We have obtained a new physical meaning to $\text{tr} \rho A$ as a number that can in principle be obtained in an appropriate single experiment, and not a mean value of many experiments which was the original physical meaning given to $\text{tr} \rho A$.

Protective measurements of different observables A_α of the first system, gives $\text{tr} \rho A_\alpha$ for each of these observables. By doing this for sufficient number of

observables, ρ may be determined. We emphasize that ρ is obtained in this way by measurements on a single system, and not by measurements on an ensemble of systems as done so far. This gives a new meaning to the density matrix by answering question (B) in the introduction affirmatively.

3 Quantum Entropy

There is an interesting difference between classical and quantum entropy. Suppose we have a gas of classical molecules in a box. If all the positions and velocities of the molecules are known then the gas cannot have a non trivial entropy. But suppose the box is now divided into many small cells and we know only which cell each molecule is in. Similarly, the velocity of each molecule is also known to some uncertainty. So, for each microstate of the gas of molecules there is a unique ‘coarse-grained’ macrostate. The entropy of any microstate is roughly the logarithm of the number of microstates which have the same macrostate as the given microstate. Thus, classically, entropy needs to be defined with respect to a coarse-grained observable. Also, this entropy is associated with an ensemble of microstates.

But quantum mechanically it is not necessary to coarse-grain in order to introduce the notion of entropy. The results of all the measurements we make on a system are determined by its density matrix ρ . If the measurements are of the usual kind, then these results are probabilities and therefore need to be given physical meaning by means of a Gibbsian ensemble of identical copies of the given system. If the measurements are protective then the results are definite values, e.g. pointer readings of the measuring apparatus, and so do not require an ensemble interpretation. But in either case, ρ completely determines the results of measurements and therefore may be regarded as a *complete* description of the system. Therefore, the quantum entropy defined in terms of ρ by

$$S = -\text{tr } \rho \ln \rho \tag{3}$$

does not require any coarse-graining. Unlike the classical entropy, quantum entropy is not defined with respect to any observable, coarse-grained or otherwise. To summarize, quantum entropy is defined using only ρ , which has the maximum possible information about the system.

A consequence of this difference is that even if the box of gas considered above is isolated from the environment, the classical entropy would remain the same or increase whereas the quantum entropy (3) remains the same because ρ undergoes unitary evolution. However, if we divide the gas into subensembles then the quantum entropy of each of them would in general increase as these subensembles become more and more entangled as a result of the interaction between the molecules. Thus quantum entropy is a measure of the degree of entanglement of the system or the impurity of the density matrix, whereas classical entropy has a very different meaning, namely it is a measure of the loss of information. E.g. if the gas of molecules were initially confined to a small part of the box, then it is overwhelmingly likely that the gas would expand to fill the box. This is accompanied by a corresponding increase in the classical entropy which represents the decrease in information of the positions of the classical molecules. But the quantum entropy of an expanding, but isolated, gas of quantum molecules remains the same because of the unitary evolution.

However, the usual interpretation of quantum entropy, like classical entropy, needs an ensemble of identical systems for its physical meaning. Because ρ can be determined by the usual measurements only statistically and therefore this is equally true for the entropy (3). Indeed, the above definition of entropy without coarse-graining has been regarded by some as possible because of the intrinsic statistical nature of quantum theory, whereas in classical physics coarse-graining, or lack of complete information, is needed to introduce the statistical element.

But the new result obtained in section 2 is that ρ may be determined by protective measurements deterministically so that ρ may be associated with

a single system. It then follows that the quantum entropy (3) also may be associated with a single system. In general, all physical quantities computed using the density matrix will from now on have a new meaning because of the new meaning to the density matrix we have given by associating it with a single system.

4 Mixtures and Fluctuations

We now turn to question (A) mentioned in the introduction, namely whether the density matrix ρ uniquely determines the state of the system. As mentioned in the previous section, ρ gives a complete description of the state of the system. Therefore, from an operational point of view, the state it describes must be unique, because two states which have the same density matrix cannot be experimentally distinguished. This conclusion seems to differ from that of d’Espagnet[4], whose arguments therefore need to be considered here.

In arguing for the possibility of different types of mixtures with the same density matrix, d’Espagnet makes a distinction between ‘proper’ and ‘improper’ mixtures. He defines a proper mixture to be a collection of μ ensembles E_1, E_2, \dots, E_μ of physical systems all of the same type with all the members of each ensemble E_α being in the same state, described say by the normalized state vector $|\phi_\alpha\rangle$. He then regards the operator

$$\rho = |\phi_\alpha\rangle \frac{N_\alpha}{N} \langle \phi_\alpha| \tag{4}$$

as the density matrix of this ‘mixture’, where $N = \sum_\alpha N_\alpha$ is the total number of elements in this collection. An improper mixture is for him the state of a subsystem of a larger system that is in a pure entangled state, which we considered in section II.

However, the above mentioned collection does not qualify to be a mixture because it does not allow for the appropriate fluctuations that a genuine mixture ought to have, and the association of the above density matrix with it

is unjustified. To illustrate the first point we shall consider the following two examples.

A famous cricketer who was leading his country's team in an international cricket test series against another country lost the toss in the first four tests. He then thought that according to the "law of chances" it is overwhelmingly likely that he would win the fifth toss, even though different coins were used for the different tosses, and so packed his team with batsmen. He lost the fifth toss too. Even more amusing is the possibly fictitious example of a man who was found carrying a bomb in a plane. When arrested he defended his action by saying "I was not planning to explode this bomb. But statisticians have told me that the probability of two passengers carrying bombs in the same plane at the same time is much smaller than the probability of just one passenger carrying a bomb. I therefore wanted to decrease the probability of someone else carrying a bomb on this plane by carrying one myself". The fallacy common to the reasoning of both men is the failure to recognize that the similar events whose probabilities are relevant here are independent.

Another way of expressing this independence is terms of fluctuations. If there are six tosses then the mean value of heads coming up is three. But of course the remaining six possible values of the number of heads can also occur, although with smaller probabilities, and they constitute the fluctuations. They ensure that even after the first four tosses turned up heads, there is an equal probability for head or tail in the fifth toss. In general, the fluctuations are such that the system has no memory. This enables thermodynamics to be possible because a thermodynamic state is described by variables such as pressure or temperature which have no memory of the history of the system.

But the 'proper mixture' as defined by d'Espagnet would have a memory: After measurements are made on n systems in the mixture, the results obtained would be relevant in predicting the probabilities of the states of the remaining $N - n$ systems, because the ratios of the numbers of systems in the various

states for the $N - n$ systems would in general be different from the ratios in the originally chosen collection of N systems. It is a memory such as this one that the above mentioned cricket captain and the bomb carrying passenger were vainly hoping for. It follows that we cannot represent the above collection of d’Espagnet by the density matrix (4) because the latter does not have this memory.

We can, however, improve on d’Espagnet’s definition of a proper mixture by taking the limit $N \rightarrow \infty$ while keeping the ratios $\frac{N}{N}$ fixed. As N becomes larger for a fixed n , the memory we have from the first n trials become correspondingly more feeble. Then the density matrix (4) will legitimately represent the limit of this sequence of collections. But it cannot be any one of this sequence, however large N may be. So, we cannot point to the state of a physical system that is represented by ρ in the sense that measurements on this state would give ρ , as d’Espagnet was trying to do, so long as only the usual measurements are performed on the system. But by doing protective measurements on a single system, as described above, we can determine ρ . To be sure there is also an idealization in the above protective measurements because they must be adiabatic. But the experiments are performed on a single system which makes them different from the usual statistical way of determining ρ by means of measurements on an ensemble of systems.

The second argument that d’Espagnet makes in support of the view that the same density matrix can represent different mixtures is the following: He states that it is possible to have different mixtures with the same density matrix that can be distinguished by their different methods of preparation. As an example he considers two methods of preparing an unpolarized beam of N spin 1/2 particles, by mixing equal amounts of particles with opposite spins with the quantization axis along the z - and x - directions respectively (ref. [4], p. 121). He claims that the density matrix is the same in both cases and it is

$$\rho = (1/2)I, \tag{5}$$

where I is the 2×2 identity matrix. He then shows correctly that the two ensembles can be experimentally distinguished by the fact that the fluctuations for the total spin in the z -direction $\Sigma_z = \sum_{n=1}^N \sigma_{z,n}$ are different for them. Because the standard deviations of this operator are 0 and \sqrt{N} for the first and second ensembles respectively.

However, as already mentioned, the results of *all* measurements on a quantum system can be obtained from its density matrix. The measurement that d’Espagnet uses to distinguish between the two ensembles is a measurement on the entire ensemble and not the individual system. If the entire ensemble is considered then the two ensembles are in different pure states and therefore obviously the corresponding density matrices are also different. So, it is not surprising that the two ensembles can be experimentally distinguished. If the individual system is considered then, as we have argued above, only in the limit of $N \rightarrow \infty$ can the ensembles have the above density matrix for the *spin* degrees of freedom. The appropriate operator for the individual system is not Σ_z , but rather the average spin in the z - direction, namely $(1/N)\Sigma_z$. The fluctuation of the latter operator is $\frac{1}{\sqrt{N}}$ which tends to zero as $N \rightarrow \infty$. So, in this limit the two mixtures for the individual spin states cannot be distinguished. This is consistent with the fact that both mixtures have the same *spin* density matrix.

But what about d’Espagnet’s claim that the two mixtures even though they have the same density matrix can in some sense be distinguished by their different methods of preparation? Actually, careful examination of his example shows that when the two pairs of beams in his example are combined, their density matrices will be different if the position variables in addition to the spin variables are taken into account. This is because of the spin position correlation in the original beams and any method of recombination must use a potential that varies with position. It is only after the position variables are traced over that the reduced density matrix has the same form (5) for the two ensembles.

But it is of course possible to obtain the same final state density matrix

starting from two different initial state density matrices by using two different Hamiltonians. This does not mean that the final states should be regarded as different. There will be no disagreement with this statement if the density matrices all describe pure states. E.g. a neutron spin state initially in the X or Y direction may be rotated to the Z direction by means of magnetic fields in Y or $-X$ directions, respectively. Although the initial states were different, the final state is the same. So, there is no reason why differently prepared states with the same density matrix should not be regarded as the same state, if the density matrix takes into account all variables. Since there is no conceivable way of distinguishing between states of a system with the same density matrix by doing only measurements on that system, we shall answer question (A) in the introduction affirmatively.

In conclusion, we have shown here that the density matrix of a mixed state is just as real as the density matrix of a pure state in that they can both be associated with the state of a single system.

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