

MEANING OF THE DENSITY MATRIX

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Received 26 December 1997; revised 27 October 1999

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. This provides a new meaning to the density matrix as having the same ontological status as the wavefunction describing a pure state. This also enables quantum entropy to be associated with a single system.

Key words: density matrix, quantum measurement, entropy.

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 mean-

ing 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. Therefore, the ensemble associated with ρ , according to the above prescription, 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. (3) The interpretation of the probabilities as relative frequencies is not possible for a fixed finite N because of fluctuations from the mean values. 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. This investigation will be primarily concerned with the following question: Can the density matrix be associated with a single system, as opposed to an ensemble? We shall answer this question affirmatively, in Sec. 2, by generalizing a method for observing a pure state by means of 'protective measurements' on a *single* system in that state [1,2] to the observation of the density matrix of a *single* system. This suggests that the density matrix may be regarded as objective and real, instead of as a catalog of probabilities for the outcomes of possible measurements. The relevance of this new meaning of the density matrix to entropy will be considered in Sec. 3. The philosophical aspects of this work will be discussed elsewhere [3].

2. PROTECTIVE MEASUREMENTS OF THE DENSITY MATRIX

A protective observation may be performed by having the observed system as a non degenerate eigenstate of the Hamiltonian and making the measurement adiabatically. Then the wave function of the system does not collapse, which makes it possible to measure several, possibly

non commuting, observables on the system. From the measurements of a sufficient number of such observables, the wave function may be reconstructed, although the measurements were all on a single system. To describe this quantitatively, write the total Hamiltonian in the form

$$H = H_A + H_S + H_I, \quad (1)$$

where H_A , H_S , and H_I are, respectively, the Hamiltonians of the apparatus, the system, and the interaction between the two. The simplest choice for H_I is the von Neumann form

$$H_I = -g(t)qA, \quad (2)$$

where A is the observable of the system that is measured, q is the observable of the apparatus that is used to monitor the state of the system, and $g(t)$ is a c-number function of time t that represents the turning on and off of the interaction. From an experimental point of view, as will become clear later, it is useful to consider the more general interaction Hamiltonian

$$H_I = -g(t) \sum_{i,j} M_{ij} q_i A_j, \quad (3)$$

where q_i , A_j are respectively observables of the system and the apparatus, M_{ij} is a non-singular constant matrix. Suppose $g(t)$ is non-zero only in the interval $(0, T)$ and

$$g_0 = \int_0^T g(t) dt. \quad (4)$$

In a protective measurement [1], g_0 is kept small and $g(t)$ is varied slowly. Then the system plus apparatus state $|\Psi\rangle$ evolves without entanglement, i.e.

$|\Psi(t)\rangle = |\chi(t)\rangle |\alpha(t)\rangle$, where χ and α are the states of the system and apparatus. And $|\chi(t)\rangle$ does not change appreciably during the measurement in $(0, T)$. Let p_i be observables of the apparatus that are conjugate to q_i , i.e. $[p_i, q_j] = -i\hbar\delta_{ij}$. On using Schrödinger's equation,

$$\frac{d}{dt} \langle \Psi | p_i | \Psi \rangle = \frac{i}{\hbar} \langle \Psi | [H, p_i] | \Psi \rangle = g(t) \sum_j M_{ij} \langle \Psi | A_j | \Psi \rangle. \quad (5)$$

Hence the changes in $\bar{p}_i \equiv \langle \Psi | p_i | \Psi \rangle = \langle \alpha | p_i | \alpha \rangle$ are

$$\Delta \bar{p}_i = \sum_j g_0 M_{ij} \langle \chi | A_j | \chi \rangle. \quad (6)$$

Thus, by observing $\Delta \bar{p}_i$, since M_{ij} is non singular, $\langle \chi | A_j | \chi \rangle$ may be obtained. Thus $\langle \chi | A_j | \chi \rangle$ are determined although only a single system is being used. By determining $\langle \chi | A_j | \chi \rangle$ for sufficient number of observables A_j on the same system, the state vector of this system $|\chi\rangle$ may be reconstructed up to a phase. Since the phase is undetermined, protective measurements really determine, even for a system that is in a pure state, its density matrix $\rho = |\chi\rangle\langle\chi|$, and not its state vector. Because this ρ was observed on a single system, it is not necessary to give it a statistical meaning.

In [1], it was assumed that the system was in an isolated non entangled state prior to its 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 observation and another system in an entangled state. Then without loss of generality the state of the combined system may be written as

$$|\chi\rangle = \sum_r c_r |\psi_r\rangle |\phi_r\rangle, \quad (7)$$

where the $\{|\psi_r\rangle\}$ and $\{|\phi_s\rangle\}$ are orthonormal sets of states of the first and the second system, respectively.

The protective observation of a state of two systems has been studied by one of us [2]. The basic ideas are: (1) Choose the interaction so that $|\chi\rangle$, that represents the state of the two systems, is a non-degenerate eigenstate of the system Hamiltonian H_S . (2) By adiabatic measurements $\{\langle \chi | A_i | \chi \rangle\}$ is determined. (3) $\{\langle \chi | A_i | \chi \rangle\}$ is sufficient to reconstruct $|\chi\rangle$ up to a phase, independently of any knowledge of H_S .

In [2], H_I was chosen so as to measure the observables of both systems so that the entangled pure state $|\chi\rangle$ could be reconstructed. But suppose now that the observable that is measured, represented by the Hermitian operator A , is that of the first system only. The interaction that protects $|\chi\rangle$ is on while this measurement is performed. Then the result of this protective measurement is

$$\langle \chi | A | \chi \rangle = \sum_r |c_r|^2 \langle \psi_r | A | \psi_r \rangle = \text{tr } \rho A, \quad (8)$$

where $\rho = \sum_r |c_r|^2 |\psi_r\rangle\langle\psi_r|$ 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 different from the protective observation of a single pure state which was studied previously [1,2]. We have now 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_i of the first system, give $\text{tr} \rho A_i$ for each of these observables. By doing this for sufficient number of observables, ρ may be determined by observations on a single system, even when ρ is impure.

As a simple example, consider as the pair of systems the spins of two particles and as the apparatus their centers of masses. Suppose that the particles have momenta \mathbf{p}_1 and \mathbf{p}_2 and equal mass m . Then

$$H_A = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m}. \quad (9)$$

Suppose also that each particle has spin 1/2, and

$$H_S = -\gamma B \mathbf{S} \cdot \mathbf{m} - \lambda \mathbf{S}_1 \cdot \mathbf{S}_2, \quad (10)$$

where $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 = \frac{1}{2}(\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)})$ is the total spin, with $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, and \mathbf{m} is a fixed unit vector. The superscripts (1) and (2) refer to operators that, respectively, act on the Hilbert spaces of the two particles. Physically, the first and second terms in H_S may correspond, respectively, to subjecting the pair of particles to a homogeneous magnetic field in the direction of \mathbf{m} and a spin-spin interaction between the particles. These interactions are so chosen in order to make all the four eigenstates of H_S non-degenerate.

Suppose that the pair of spins is in an eigenstate of H_S . We now subject the first particle to a Stern-Gerlach magnetic field for which the interaction Hamiltonian is

$$H_I = -\mu g(t) \sum_{i,j} L_{ij} x_j^{(1)} \sigma_i^{(1)}, \quad (11)$$

where L_{ij} is a known non singular matrix. L_{ij} is required to be symmetric and traceless in order that the magnetic field $B_i = \sum_j L_{ij} x_j$ satisfy the Maxwell's equations¹ $\text{div} \mathbf{B} = 0$ and $\text{curl} \mathbf{B} = 0$. Suppose also that the measurement is adiabatic with respect to the time scale $\hbar/\Delta E$, where $\Delta E > 0$ is the smallest separation among the eigenvalues of H_S . Then the inhomogeneous magnetic field would not split the wave packet. And the change of the mean values of the momenta p_j conjugate to x_j , using (6), are

$$\Delta \bar{p}_j = g_0 \mu \sum_i L_{ij} \sum_{r=1}^2 |c_r|^2 \langle \psi_r | \sigma_i^{(1)} | \psi_r \rangle = g_0 \mu \sum_i L_{ij} \text{tr} \rho \sigma_i^{(1)}, \quad (12)$$

¹The often made simplifying assumption that L_{ij} are zero except for one diagonal element implies that $\text{div} \mathbf{B} \neq 0$. It is for this reason that the above L_{ij} was used in (11), and the matrix M_{ij} was introduced in (3).

where ρ is the reduced density matrix of the spin degree of freedom of the first particle.

Hence, by measuring $\Delta\bar{p}_i$, we can determine $\text{tr}\rho\sigma_i^{(1)}$. Since, ρ is a 2×2 Hermitian matrix with $\text{tr}\rho = 1$, ρ depends on three real parameters. Therefore, by measuring $\Delta\bar{p}_j, j = 1, 2, 3$, ρ may be determined from a single experiment. For instance, we may write

$$\rho = \sum_{j=1}^3 a_j \sigma_j^{(1)} + \frac{1}{2}I,$$

where a_j are real. Then $\text{tr}\rho\sigma_i^{(1)} = a_i$. Hence by measuring $\Delta\bar{p}_i$, a_i and therefore ρ is uniquely determined.

It is important to note that during these measurements the projective interaction given by H_S should be on. Otherwise the wave packet would split into the eigenstates of $\sum_i L_{ij}\sigma_i^{(1)}$ like in the usual Stern-Gerlach experiment. Then $\Delta\bar{p}_j$ would have two possible outcomes corresponding to these two eigenstates. We observe only one of these two possibilities, and this outcome may only be predicted probabilistically. The density matrix ρ then needs to be determined by experiments on an ensemble, and ρ would therefore have a statistical meaning. In contrast, in the above described protective measurement there is only one possible deterministic outcome for $\Delta\bar{p}_j$. Therefore, ρ may be obtained in this way by measurements on a single system, instead of by measurements on an ensemble of systems. This gives a new meaning to the density matrix by answering the question in the introduction affirmatively.

3. QUANTUM ENTROPY

There are two ways of defining classical and quantum entropy. Suppose we have a gas of classical molecules in a box. According to the first definition that we shall discuss, 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 macrostate is the logarithm of the number of microstates which have the given macrostate. Thus this entropy is defined with respect to a coarse-grained observable, and will be called coarse-grained entropy. Also, this entropy is associated with an ensemble of microstates.

But in quantum mechanics, entropy maybe introduced without coarse-graining. The results of all the measurements we could 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, as described earlier, then the results are definite values, e.g., pointer readings of the measuring apparatus, and so do not require an ensemble interpretation. 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

$$S = -k \operatorname{tr} \rho \ln \rho, \quad (13)$$

where k is Boltzmann's constant, does not require any coarse-graining. Unlike the coarse-grained entropy, the above 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 coarse-grained entropy would remain the same or increase whereas the quantum entropy (13) 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 with the environment or the impurity of its density matrix, whereas coarse-grained 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 coarse-grained 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 coarse-grained entropy, needs an ensemble of identical systems for its physical meaning. This is because ρ can be determined by the usual measurements only statistically and therefore this is equally true for the entropy (13). Indeed, this 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 Sec. 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 en-

tropy (13) also may be associated with a single system. Therefore, the entropy need not be given the usual statistical meaning, that acquires physical meaning through an ensemble. But instead the entropy may be regarded as a measure of the degree of entanglement of an individual system with its environment. In general, all physical quantities computed using the density matrix will from now on have a new meaning of being associated with a single system because of the new meaning to the density matrix we have given by associating it with a single system.

Acknowledgements. We thank Katherine Brading for stimulating discussions. This work was supported by NSF grant PHY-9601280 and the work of Y.A. by the Israel National Academy of Sciences under grant no. 61495.

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