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Quantum mechanics without state vectors

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Because the state vectors of isolated systems can be changed in entangled states by processes in other isolated systems, keeping only the density matrix fixed, it is proposed to give up the description of physical states in terms of ensembles of state vectors with various probabilities, relying only on density matrices. The density matrix is defined here by the formula giving the mean values of physical quantities, which implies the same properties as the usual definition in terms of state vectors and their probabilities. This change in the description of physical states opens up a large variety of new ways that the density matrix may transform under various symmetries, different from the unitary transformations of ordinary quantum mechanics. Such new transformation properties have been explored before, but so far only for the symmetry of time translations into the future, treated as a semigroup. Here, new transformation properties are studied for general symmetry transformations forming groups, not just semigroups. Arguments that such symmetries should act on the density matrix as in ordinary quantum mechanics are presented, but all of these arguments are found to be inconclusive.

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I. A MODEST PROPOSAL

One of the most disturbing aspects of quantum mechanics arises from entanglement [1]. In an entangled state in ordinary quantum mechanics an intervention in the state vector affecting one part of a system can instantaneously affect the state vector describing a distant isolated part of the system. It is true that in ordinary quantum mechanics no measurement in one subsystem can reveal what measurement was done in a different isolated subsystem, but the susceptibility of the state vector to instantaneous change from a distance casts doubts on its physical significance.

Entanglement is much more of a problem in some modifications of quantum mechanics that are intended to resolve the problem of measurement, such as the general nonlinear stochastic evolution studied in [2]. It is difficult in these theories even to formulate what we mean by isolated subsystems, much less to prevent instantaneous communication between them [3,4]. Polchinski [4] has shown that unless nonlinearities are constrained to depend only on the density matrix, such modified versions of quantum mechanics even allow communication between the different worlds of the many-worlds description of quantum mechanics.

The problem of instantaneous communication between distant isolated systems has been nicely summarized in a theorem of Gisin [3]. It states that in a system consisting of two isolated subsystems *I* and *II*, with a prescribed density matrix ρ^I for subsystem *I*, it is always possible in a suitable entangled state of the two subsystems to make measurements on subsystem *II* that put subsystem *I* in *any* set of states Ψ_r^I (not necessarily orthogonal) with any probabilities P_r, provided only that $\sum_r P_r \Lambda_r^I = \rho^I$, where Λ_r^I is the projection operator on the state Ψ_r^I. Since any statement that a system is in an ensemble of states with definite probabilities can thus be changed instantaneously by a measurement at an arbitrary distance, keeping only the density matrix fixed, it seems reasonable to infer that such statements are meaningless, and that only the density matrix has meaning.

Taking the density matrix as the description of physical states is very different from giving the same status to an ensemble of state vectors with various probabilities because the density matrix contains much less information. If we know that a system is in any one of a number of states Ψ_r, with probabilities P_r, then we know that the density matrix is $\rho = \sum_r P_r \Lambda_r$, where Λ_r is the projection operator on state Ψ_r, but this does not work in reverse. As is well known, for a given density matrix ρ there are any number of ensembles of not necessarily orthogonal or even independent state vectors and their probabilities that give the same density matrix. (An exception is discussed in Sec. II.) The density matrix is of course a Hermitian operator on Hilbert space, a vector space. In speaking of "quantum mechanics without state vectors" I mean only that a statement that a system is in any one of various state vectors with various probabilities is to be regarded as having no meaning, except for what it tells us about the density matrix [5].

For example, suppose the density matrix of a spin-$\frac{1}{2}$ particle, in a basis provided by states with the north component of spin equal to $+\frac{1}{2}$ or $-\frac{1}{2}$, takes the form

$$\rho = \begin{pmatrix} 0.69 & 0.17 \\ 0.17 & 0.31 \end{pmatrix}.$$

By diagonalizing this matrix, we might conclude that this particle has a 75% probability of being in a pure state with spin pointing northeast and a 25% probability of being in an orthogonal pure state with spin pointing southwest. But, we get the same density matrix if the particle has a 50% probability of being in a pure state with spin pointing north, a 15% probability of being in a pure state with spin pointing south, and a 35% probability of being in a pure state with spin pointing east. These two ensembles sound different, but in fact they are indistinguishable. Indeed, they had better be indistinguishable because otherwise we could communicate instantaneously at an arbitrary distance by acting on a distant isolated system with which this particle's state vector is entangled so as to change the spin states from the first to the second ensemble. It is better just to specify the density matrix, and give up its description in terms of an ensemble of state vectors with various probabilities.

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If the density matrix is not to be defined in terms of ensembles of state vectors, then what is it? We may define it by postulating a physical interpretation: The average value $\overline{A}$ of any physical quantity represented by a Hermitian operator A is $\mathrm{Tr}(A\rho)$, which since it applies also to powers of A allows us to find from the density matrix the probability distribution for values of the quantity represented by A. This postulate leads to all the properties of the density matrix that are usually derived from its interpretation in terms of an ensemble of state vectors with various probabilities. The density matrix must be Hermitian in order that $\mathrm{Tr}(A\rho)$ should be real for an arbitrary Hermitian operator A. The density matrix must have unit trace in order that $\mathrm{Tr}(\alpha\rho)=\alpha$ for any c number α. The density matrix must be positive in order that $\mathrm{Tr}(A\rho)$ should be positive for any positive Hermitian operator A. Also, a physical quantity represented by a Hermitian operator A will have a definite value α (in the sense that the mean value of A^n is α^n for all integers n) if and only if $A\rho=\alpha\rho$.

It may seem like a mere matter of language to say that it is the density matrix rather than an ensemble of state vectors with various probabilities that should be taken as the description of a physical system. Already, many studies of the interpretation of quantum mechanics and of quantum information theory are based on the density matrix rather than the state vector, without needing a new interpretation of quantum mechanics. What difference does it make?

There is one big difference, which is our chief concern in this paper. Giving up the definition of the density matrix in terms of state vectors opens up a much larger variety of ways that the density matrix might respond to various symmetry transformations. In ordinary quantum mechanics, a symmetry transformation takes a density matrix ρ into $U\rho U^\dagger$, where U is a unitary (or, for time reversal, antiunitary) operator belonging to one of the representations of the symmetry group. This is certainly not the only way that a Hermitian matrix could transform. For instance, we may consider a system with an SU(3) symmetry and a Hilbert space of three dimensions, in which the density matrix transforms under SU(3) as the reducible representation $3+\overline{3}+1+1+1$. In a suitable basis, we would have

$$\rho=\begin{pmatrix} a_1 & b_3 & b_2^* \\ b_3^* & a_2 & b_1 \\ b_2 & b_1^* & a_3 \end{pmatrix},$$

where under SU(3) the real diagonal elements a_n transform as singlets, with $a_1+a_2+a_3=1$, and the triplet (b_1,b_2,b_3) transforms as the representation 3. This SU(3) transformation of ρ cannot be put in the form $\rho\mapsto U\rho U^\dagger$ required in ordinary quantum mechanics because if the 3×3 matrix U belonged to the representations 3 or $\overline{3}$, then ρ would transform as $3\times\overline{3}=1+8$, not $3+\overline{3}+1+1+1$. (The other possibility is that U belongs to the representation $1+1+1$, in which case ρ would transform as a sum of singlets, again not including $3+\overline{3}$.) The question of the positivity of a density matrix transforming in this way is discussed in Sec. VII.

The possibility of an unusual transformation of the density matrix has been widely considered, but up to now I believe only for the symmetry of time translation. In this case, it is known that the evolution of the density matrix with time is in general governed by a first-order linear differential equation, such as the Lindblad equation [6] (given here in Sec. VIII), different from what is found in ordinary quantum mechanics. The Lindblad equation is commonly used to study open systems in ordinary quantum mechanics, with the effects of the environment integrated out, but it has also been used to deal with the problem of measurement [7] in closed systems. A stochastic evolution of the state vector can be arranged to yield a Lindblad equation for the density matrix, and with a suitable choice of the details of this differential equation, its solutions can reproduce the results of measurement according to the Copenhagen interpretation, but through a smooth spontaneous localization of the density matrix [7] rather than a sudden intrusion of classical physics. (These matters are discussed in a separate paper [8].) These theories share the well-known feature of ordinary quantum mechanics, that entanglement does not lead to communication at a distance between isolated systems. This is because (as explained in Sec. III, in a more general context) nothing that is done in one system can instantaneously affect the density matrix of another isolated system, although it can affect the state vector. Also, all predictions can be derived from the density matrix, without knowing anything about state vectors, and the evolution of the density matrix in these theories depends only on the density matrix, not on the state vector. But, from the point of view explored in the present work, the study of the stochastic evolution of the state vector is unnecessary; it is only the differential equation for the density matrix that matters.

The time-translation symmetry transformations used in deriving the Lindblad equation take us only into the future, not the past, and hence form a semigroup, not a group. If we are willing to consider new ways that the density matrix might transform under time translation, then we ought to do the same for general symmetry groups, not just semigroups.

This proposal runs into potential difficulties, each of which can be escaped through a narrow loophole. As shown in Sec. II, in order to allow for any new group transformation rules, we would need to restrict the class of Hermitian operators that represent physical quantities. In order for the transformation of the density matrix under a continuous symmetry group to take a form different from that of ordinary quantum mechanics, it would also be necessary to restrict the class of physically realizable density matrices, as described in Sec. VII. Finally, using a requirement related to the condition of complete positivity, it is shown in Sec. VIII that the same applies to discrete symmetry groups. If further study shows that these loopholes are not actually open, then on the basis of the arguments of this paper, we could conclude that, even in a quantum mechanics without state vectors, the density matrix must transform under symmetry groups just as in ordinary quantum mechanics.

II. PHYSICAL QUANTITIES AND UNUSUAL SYMMETRIES

To explore unusual possibilities for symmetry transformations, we need first to say what we mean by a symmetry transformation. We will take a symmetry transformation to be a linear mapping $\rho\mapsto g(\rho)$ of density matrices, which preserve their Hermiticity, positivity, and unit trace. For

any such transformation g, we further assume that there is a corresponding linear transformation $A \mapsto g(A)$ of any Hermitian operator A representing a physical quantity, which preserves its Hermiticity, such that the mean value of the physical quantity is left invariant:

$$\mathrm{Tr}[g(A)\, g(\rho)] = \mathrm{Tr}(A\, \rho). \tag{1}$$

With this definition of symmetry transformations, it is important to decide just what operators can represent physical quantities. Certainly, we want to include familiar quantities such as momentum, angular momentum, etc., and functions of these quantities. In particular, the projection operator on a nondegenerate eigenstate of such a physical quantity, as for instance the projection operator $(1 \pm 2s_z)/2$ on a state of a spin $\frac{1}{2}$ with $s_z = \pm\frac{1}{2}$, represents a physical quantity. In ordinary quantum mechanics, *any* Hermitian operator is assumed to represent a physical quantity, but if state vectors are not to be taken as a representation of reality, we can doubt whether operators Λ_Ψ that are defined as the projection operators on arbitrary state vectors Ψ necessarily represent physical quantities. If they did, then according to our interpretive postulate $\mathrm{Tr}(\Lambda_\Psi\, \rho)$ would be the probability that a system with density matrix ρ is in a state Ψ, which is just the sort of statement that we are here taking as generally meaningless. In any case, it is hard to see how one could ever tell that Schrödinger's cat is in a state $|\mathrm{alive}\rangle + |\mathrm{dead}\rangle$ rather than, say, $|\mathrm{alive}\rangle - |\mathrm{dead}\rangle$.

This point is important for us because if all Hermitian operators including projection operators represent physical quantities, then with our assumptions it can be shown that density matrices transform under any symmetry transformation g with an inverse just as in ordinary quantum mechanics [9]:

$$g(\rho) = U\, \rho\, U^\dagger, \tag{2}$$

with U unitary or antiunitary.

The first step in the proof is to show that if all projection operators are physical quantities in the above sense, then any symmetry transformation g with an inverse g^{-1} takes any projection operator Λ (defined here as a Hermitian operator with $\Lambda^2 = \Lambda$ and $\mathrm{Tr}\Lambda = 1$) into another projection operator. According to our definition of symmetries, any density matrix ρ is mapped into a Hermitian positive matrix $g(\rho)$ with unit trace, which can therefore be expressed as

$$g(\rho) = \sum_n P_n \Lambda_n,$$

where Λ_n are projection operators, satisfying $\Lambda_n \Lambda_m = \delta_{nm}\Lambda_n$ and $\mathrm{Tr}\Lambda_n = 1$, and the P_n are positive real numbers with $\sum_n P_n = 1$. We then have

$$\rho = \sum_n P_n\, g^{-1}(\Lambda_n).$$

If all projection operators represent physical quantities, then we can use Eq. (1) with any Λ_n in place of A, ρ taken as any Λ_m, and g replaced with g^{-1}, so that

$$\mathrm{Tr}[g^{-1}(\Lambda_n)\, g^{-1}(\Lambda_m)] = \mathrm{Tr}(\Lambda_n\, \Lambda_m) = \delta_{nm}.$$

Hence,

$$\mathrm{Tr}(\rho^2) = \sum_n P_n^2.$$

Now, if ρ is a projection operator, then $\rho^2 = \rho$, so $\mathrm{Tr}(\rho^2) = \mathrm{Tr}(\rho) = 1$, and therefore $\sum_n P_n^2 = 1$. But the only way that this can be satisfied by a set of real positive numbers P_n with $\sum_n P_n = 1$ is to have all P_n vanish except for one, say P_1, with the value $P_1 = 1$. Then, $g(\rho)$ is itself a projection operator, namely Λ_1.

The rest of the proof is completed quickly. Any projection operator Λ can be expressed as a dyad $\Lambda_\Psi = \Psi\Psi^\dagger$, where Ψ is a normalized state vector, unique up to a phase. (This is the exception mentioned in Sec. I to the rule that density matrices may be expressed in various different ways as linear combinations of projection operators; the only such representation of a projection operator is as a unique dyad.) Since as we have seen any symmetry transformation g with an inverse takes projection operators into projection operators, we must have $g(\Lambda_\Psi) = \Lambda_{g(\Psi)}$, where the state vector $g(\Psi)$ is unique up to a phase. Again, if these projection operators are all to be taken as representing physical quantities, then in Eq. (1) we can take $A = \Lambda_\Psi$ and $\rho = \Lambda_\Phi$ for any two state vectors Ψ and Φ, and find

$$\mathrm{Tr}(\Lambda_{g(\Psi)}\, \Lambda_{g(\Phi)}) = \mathrm{Tr}(\Lambda_\Psi\, \Lambda_\Phi)$$

and therefore

$$|(g(\Psi), g(\Phi))|^2 = |(\Psi, \Phi)|^2.$$

According to Wigner's theorem [10], if this condition is satisfied for all normalized state vectors Φ and Ψ (which from our present point of view does not need to be assumed), then it must be possible to choose the phases of all $g(\Psi)$ so that

$$g(\Psi) = U_g \Psi,$$

where U_g is a unitary (or antiunitary) operator, the same for all Ψ. In this case, we have $g(\Lambda_\Psi) = U_g \Lambda_\Psi U_g^\dagger$. Since any density matrix can be expressed (though not uniquely) as a linear combination of projection operators, they also transform as in Eq. (2), as was to be proved.

We thus have a choice. We can assume that the invariance condition (1) holds for all density matrices ρ and all Hermitian operators A, in which case density matrices can only have the same transformation properties (2) as in ordinary quantum mechanics. Or, we can limit the validity of Eq. (1) to a class of physical quantities that does not include projection operators on every state vector, in which case density matrices may have a much wider variety of symmetry transformation properties. In this paper, we will explore the consequences of the latter choice.

The behavior of the density matrix under general symmetry transformations is outlined here in Sec. III. In Sec. IV, these general results are applied and further explored for the case of continuous symmetries. The group multiplication law is found to impose severe constraints on the transformation of the density matrix. Section V presents an example of a class of continuous symmetries whose action on the density matrix explicitly satisfies these constraints, but is different from the transformation found in ordinary quantum mechanics.

Section VI describes special features of the action of compact groups on the density matrix. Section VII takes up the important but difficult question of deciding what conditions should be imposed on the transformation of the density matrix under general symmetry operations so that these transformations will preserve the positivity of the density matrix. Section VIII shows that assuming the positivity of the eigenvalues of the transformation kernel rules out the possibility that the density matrix transforms differently than in ordinary quantum mechanics, and suggests a reason why these eigenvectors need not be positive.

III. GENERAL SYMMETRIES

We suppose that a general element g of the symmetry group of a system induces on the density matrix a linear transformation $\rho \mapsto g(\rho)$, with

$$g(\rho)_{M'N'} = \sum_{MN} K_{M'M,N'N}[g]\,\rho_{MN}, \tag{3}$$

where $K[g]$ is some c-number kernel independent of ρ. We will take the indices M, N, etc. to run here over a finite number d of values, but will assume that the formalism can be extended to Hilbert spaces of infinite dimensionality, on which the matrices considered here become well-behaved operators. (No attempt will be made here to apply this formalism to relativistic theories [11].) Our reason for concentrating on linear transformations is explained later in this section.

In order for $g(\rho)$ to be Hermitian for an arbitrary Hermitian ρ, it is necessary and sufficient that K be Hermitian, in the sense that

$$K_{M'M,N'N}[g]^* = K_{N'N,M'M}[g]. \tag{4}$$

(This is why it proves convenient to put the subscripts on $K[g]$ in what may otherwise look like a peculiar order.) Also, in order for $g(\rho)$ to have unit trace for an arbitrary ρ with unit trace, it is necessary and sufficient that

$$\sum_{M'} K_{M'M,M'N}[g] = \delta_{MN}. \tag{5}$$

The difficult thing is to know what additional conditions should be imposed on $K[g]$ (or on ρ) so that $g(\rho)$ will be positive. This will be discussed in Secs. VII and VIII.

The great physical advantage of basing quantum mechanics on the density matrix, with linear symmetry transformation properties, is that the transformation properties of the density matrix for an isolated subsystem do not depend on the properties of any other distant isolated subsystem, even in the case of entanglement, where the density matrix does not factorize into density matrices for the individual subsystems. Suppose that the system consists of two parts, subsystems *I* and *II*, which are isolated in the sense that no physical influence and no message can pass from one to the other. We replace the indices M, N, etc. with compound indices ma, nb, etc., with the first letter labeling the states of subsystem *I* and the second the states of subsystem *II*. The possibility of entanglement does not in general allow the density matrix to factor into a product $\rho^{(I)}_{mn}\rho^{(II)}_{ab}$ of density matrices for the two subsystems, but if the subsystems are isolated they transform independently, in the sense that the kernel in Eq. (3) does factorize:

$$K_{m'a'ma,n'b'nb}[g] = K^{(I)}_{m'm,n'n}[g]\; K^{(II)}_{a'a,b'b}[g], \tag{6}$$

where $K^{(I)}[g]$ and $K^{(II)}[g]$ are the kernels that would describe the transformation of the density matrix in subsystems *I* and *II* if the other subsystem did not exist. Equation (6) is true in particular for the transformation (2) of ordinary quantum mechanics, if the generator T of this transformation (such as the Hamiltonian in the case of time translation) is a sum $T = T^{(I)} + T^{(II)}$ of operators $T^{(I)}$ and $T^{(II)}$ that act respectively only on the indices $m,n,\ldots$ and $a,b,\ldots$. Here, we are taking Eq. (6) as the characteristic feature of isolated systems even for more general transformation rules. [For a nonlinear transformation it would be difficult to see what could take the place of Eq. (6) as a statement of what we mean by *isolated* subsystems.] Since both $K^{(I)}[g]$ and $K^{(II)}[g]$ are possible physical kernels, they each satisfy the analog of Eq. (5):

$$\sum_{m'} K^{(I)}_{m'm,m'n}[g] = \delta_{mn}, \quad \sum_{a'} K^{(II)}_{a'a,a'b}[g] = \delta_{ab}. \tag{7}$$

The density matrix of subsystem *I* is related to the density matrix of the whole system by

$$\rho^{(I)}_{mn} = \sum_a \rho_{ma,na}. \tag{8}$$

[This follows from the requirement that the mean value $\mathrm{Tr}(\rho A)$ of any physical quantity represented by an operator of the form $A_{ma,nb} = A^{(I)}_{mn}\delta_{ab}$, which acts nontrivially only on subsystem *I*, should be equal to $\mathrm{Tr}(\rho^{(I)}A^{(I)})$.] According to Eqs. (3), (6), and (8), its transformation is given by

$$\begin{aligned}\rho^{(I)}_{m'n'} &\mapsto g^{(I)}(\rho)_{m'n'}\\ &= \sum_{a'}\sum_{mnab} K^{(I)}_{m'm,n'n}[g]\; K^{(II)}_{a'a,a'b}[g]\;\rho_{ma,nb}.\end{aligned}$$

Using Eq. (7) for $K^{(II)}$ and Eq. (8) again, this is

$$g^{(I)}(\rho)_{m'n'} = \sum_{mn} K^{(I)}_{m'm,n'n}[g]\;\rho^{(I)}_{mn}, \tag{9}$$

so the transformation of $\rho^{(I)}$ is independent of $\rho^{(II)}$. This applies in particular to the symmetry of time translation, so as well known even in entangled states the evolution of the density matrix for subsystem *I* is unaffected by whatever happens in an isolated subsystem *II*.

Now, let us return to the general case, and our former notation. Because the kernel $K[g]$ is Hermitian in the sense of Eq. (4), it can be expanded as

$$K_{M'M,N'N}[g] = \sum_i \eta^{(i)}[g]\; u^{(i)}_{M'M}[g]\; u^{(i)*}_{N'N}[g], \tag{10}$$

where the $u^{(i)}_{M'M}[g]$ and $\eta^{(i)}[g]$ are a complete set of normalized eigenmatrices and eigenvalues of the kernel $K_{M'M,N'N}[g]$, in the sense that

$$\sum_{N'N} K_{M'M,N'N}[g]\, u^{(i)}_{N'N}[g] = \eta^{(i)}[g]\, u^{(i)}_{M'M}[g], \tag{11}$$

$$\mathrm{Tr}(u^{(i)\dagger}[g]\, u^{(j)}[g]) = \delta_{ij}. \tag{12}$$

[Note that Eq. (11) does *not* say that the map (3) takes $u^{(i)}[g]$ into $\eta^{(i)}[g]\,u^{(i)}[g]$.] The transformed density matrix (3) can then be written more compactly as a sum of matrix products:

$$g(\rho) = \sum_i \eta^{(i)}[g]\; u^{(i)}[g]\; \rho\; u^{(i)\dagger}[g]. \tag{13}$$

The trace condition (5) here reads as

$$\sum_i \eta^{(i)}[g]\; u^{(i)\dagger}[g]\; u^{(i)}[g] = \mathbf{1}, \tag{14}$$

where $\mathbf{1}$ is the unit matrix. If there were only one eigenvector $u^{(1)}[g]$ with a nonzero eigenvalue $\eta^{(1)}[g]$, then Eq. (14) would require $\eta^{(1)}[g] > 0$, and the transformation rule (13) could be written $g(\rho) = U[g]\;\rho\;U^\dagger[g]$, where according to Eq. (14) the matrix $U[g] \equiv \sqrt{\eta^{(1)}[g]}u^{(1)}[g]$ appearing in this transformation rule is unitary. But, in the general case, where the kernel has several independent eigenmatrices with nonzero eigenvalues, Eqs. (13) and (14) represent a nontrivial generalization of the unitary transformations of ordinary quantum mechanics.

We also need to impose on $K[g]$ the group property, that for any two symmetry transformations g and $\overline{g}$, we have

$$\sum_{M'N'} K_{M''M',N''N'}[g]\; K_{M'M,N'N}[\overline{g}] = K_{M''M,N''N}[g\overline{g}]. \tag{15}$$

(This condition is not usually mentioned in connection with time translation because, as we shall see, it does not constrain the differential equation that governs the temporal evolution of the density matrix, but it does need to be imposed even for time translation when that symmetry is combined with other symmetries.) Using the representation (10), the group property (15) may be written

$$\sum_{M'N'}\sum_{ij} \eta^{(i)}[g]\,\eta^{(j)}[\overline{g}]\,u^{(i)}_{M''M'}[g]\,u^{(j)}_{M'M}[\overline{g}]\,u^{(i)\dagger}_{N'N''}[g]\,u^{(j)\dagger}_{NN'}[\overline{g}]$$
$$= \sum_k \eta^{(k)}[g\overline{g}]\,u^{(k)}_{M''M}[g\overline{g}]\,u^{(k)\dagger}_{NN''}[g\overline{g}] \tag{16}$$

or, in an abbreviated notation,

$$\sum_{ij} \eta^{(i)}[g]\,\eta^{(j)}[\overline{g}]\,u^{(i)}[g]\,u^{(j)}[\overline{g}]\otimes u^{(j)\dagger}[\overline{g}]\,u^{(i)\dagger}[g]$$
$$= \sum_k \eta^{(k)}[g\overline{g}]\,u^{(k)}[g\overline{g}]\otimes u^{(k)\dagger}[g\overline{g}], \tag{17}$$

it being understood that for any two $d\times d$ matrices A and B,

$$[A\otimes B]_{M'M,N'N} \equiv A_{M'M}\;B_{NN'}. \tag{18}$$

In the next section, we will explore the implications of Eq. (17) for continuous symmetries.

IV. CONTINUOUS SYMMETRIES

We now consider a group of transformations that includes elements arbitrarily close to the identity $\mathbf{I}$. For the identity, we have of course

$$K_{M'M,N'N}[\mathbf{I}] = \delta_{M'M}\delta_{N'N}. \tag{19}$$

This has one eigenmatrix $u^{(1)}[\mathbf{I}]$ with nonzero eigenvalue

$$u^{(1)}_{N'N}[\mathbf{I}] = \delta_{N'N}/\sqrt{d}, \quad \eta^{(1)}[\mathbf{I}] = d, \tag{20}$$

and d^2-1 eigenmatrices $u^{(\alpha)}[\mathbf{I}]$, a complete set of traceless matrices, all with eigenvalues zero:

$$\mathrm{Tr}\; u^{(\alpha)}[\mathbf{I}] = 0, \quad \eta^{(\alpha)}[\mathbf{I}] = 0. \tag{21}$$

Now, let us consider group elements $g(\epsilon n)$, with $g(0) = \mathbf{I}$, where ϵ is infinitesimal, and n^r is a real vector specifying a fixed direction in the space of group parameters near the origin. The kernel $K[g(\epsilon n)]$ may be supposed to be analytic in ϵn for ϵn near zero, but because the eigenvalues $\eta^{(\alpha)}[g(\epsilon n)]$ are degenerate for $\epsilon = 0$, according to the familiar rules of first-order perturbation theory the corresponding unperturbed eigenmatrices must be chosen to diagonalize the first-order perturbation to $K[g(\epsilon n)]$, and therefore may remain functions of the direction (but not of the magnitude) of n even for $\epsilon \to 0$. That is, in the limit $\epsilon \to 0$, the $u^{(\alpha)}[g(\epsilon n)]$ approach $u^{(\alpha)}(n)$, where

$$\sum_{M'MN'N} u^{(\alpha)*}_{M'M}(n)\left[\frac{\partial K_{M'M,N'N}[g(\epsilon n)]}{\partial\epsilon}\right]_{\epsilon=0} u^{(\beta)}_{N'N}(n)$$
$$= \delta_{\alpha\beta}\;\Delta^{(\alpha)}(n), \tag{22}$$

where $\Delta^{(\alpha)}(n)$ scales as $\Delta^{(\alpha)}(cn) = c\Delta^{(\alpha)}(n)$, but like $u^{(\alpha)}(n)$ is not in general analytic in n at $n = 0$. To first order in ϵ, the corresponding eigenvalues are

$$\eta^{(\alpha)}[g(\epsilon n)] \to \epsilon\;\Delta^{(\alpha)}(n). \tag{23}$$

On the other hand, the eigenvalue $\eta^{(1)}[g(\epsilon n)]$ is not degenerate and does not vanish for $\epsilon = 0$, so the quantity $\sqrt{\eta^{(1)}[g(\epsilon n)]}u^{(1)}[g(\epsilon n)]$, which appears in the terms in Eq. (10) with i or j or k equal to 1, may be supposed to be given by a power series in ϵn:

$$\sqrt{\eta^{(1)}[g(\epsilon n)]}u^{(1)}[g(\epsilon n)] \to 1 - i\epsilon\; n\cdot\tau + O(\epsilon^2), \tag{24}$$

with $n\cdot\tau \equiv \sum_r n^r\tau_r$, where $[\tau_r]_{N'N}$ are constant matrices (not necessarily Hermitian), independent of ϵ and n.

The trace condition (14) tells us the anti-Hermitian parts of the matrices τ_r:

$$-in\cdot\tau + in\cdot\tau^\dagger + \sum_\alpha \Delta^{(\alpha)}(n)\,u^{(\alpha)\dagger}(n)u^{(\alpha)}(n) = 0. \tag{25}$$

This shows that although $\Delta^{(\alpha)}(n)$ and $u^{(\alpha)\dagger}(n)$ are complicated functions of the vector n that defines a infinitesimal group element, the sum in Eq. (25) is simply linear in the components of n, and since it is Hermitian, we can write

$$\sum_\alpha \Delta^{(\alpha)}(n)\,u^{(\alpha)\dagger}(n)u^{(\alpha)}(n) = \sum_r n^r\theta_r, \tag{26}$$

where θ_r is Hermitian and independent of n. We therefore have

$$\tau_r = T_r - \frac{i}{2}\theta_r, \tag{27}$$

where T_r too is Hermitian.

Using these results in Eq. (13), we find the first-order change in the density matrix due to the transformation $g[\epsilon n]$:

$$\delta_{\epsilon n}\rho = i\epsilon\,[n\cdot T,\rho] + \epsilon\sum_\alpha \Delta^{(\alpha)}(n)\left[u^{(\alpha)}(n)\,\rho\,u^{(\alpha)\dagger}(n)\right.$$
$$\left. - \frac{1}{2}u^{(\alpha)\dagger}(n)u^{(\alpha)}(n)\,\rho - \frac{1}{2}\rho\,u^{(\alpha)\dagger}(n)u^{(\alpha)}(n)\right]. \tag{28}$$

It is the set of matrices T_r that here play a role like the usual Hermitian matrix representation of the Lie algebra, although as we shall see it is only in special cases that they can be shown to satisfy the same commutation relations.

We can use Eq. (28) to find the effect of any infinitesimal symmetry transformation g on any physical quantity represented by an operator A. Writing $g(A) = A + \delta_{\epsilon n} A$, to first order in ϵ Eq. (1) gives

$$\mathrm{Tr}(\delta_{\epsilon n} A\ \rho) = -\mathrm{Tr}(A\ \delta_{\epsilon n}\rho). \tag{29}$$

For this to hold for all density matrices ρ, we must have

$$\delta_{\epsilon n} A = i\epsilon\,[n\cdot T, A] - \epsilon \sum_\alpha \Delta^{(\alpha)}(n)\left[u^{(\alpha)\dagger}(n)\,A\,u^{(\alpha)}(n) - \frac{1}{2}u^{(\alpha)\dagger}(n)u^{(\alpha)}(n)\,A - \frac{1}{2}A\,u^{(\alpha)\dagger}(n)u^{(\alpha)}(n)\right]. \tag{30}$$

In particular, the physical quantity represented by A is invariant under this symmetry if $\delta_{\epsilon n} A$ vanishes. Unlike the density matrix, this quantity is invariant if (although perhaps not only if) A commutes with $T\cdot n$ and with all $u^{(\alpha)}(n)$. In this case, all powers of A and hence the whole probability distribution of A are also invariant.

It may be noted that in itself the transformation rule (28) does not uniquely fix the matrices T_r and $u^{(\alpha)}(n)$. Without changing $\delta_{\epsilon n}\rho$, we may shift these matrices by

$$\begin{aligned}\Delta\, u^{(\alpha)}(n) &= \mathbf{1}\,\mathrm{Tr}[C u^{(\alpha)}(n)],\\ [\Delta\, T_r]_{M'M} &= \frac{i}{2}\sum_{N'N}[L_r]_{M'M,NN'}C_{N'N} - \frac{i}{2}\sum_{N'N}[L_r]^*_{MM',NN'}C^*_{N'N},\end{aligned}$$

where C is an arbitrary complex matrix. This allows us to make the trace of $u^{(\alpha)}(n)$ anything we like, for if we take $C = \sum c_\beta u^{(\beta)\dagger}(n)$ with c_β arbitrary, then [using Eq. (12)] we have $\mathrm{Tr}[\Delta u^{(\alpha)}(n)] = c_\alpha d$. However, in this paper we will stick to the original definitions of T_r and $u^{(\alpha)}(n)$, characterized by the tracelessness of $u^{(\alpha)}(n)$.

So far, this section has closely followed the usual treatment of the symmetry of time translation, especially as in Ref. [12]. This symmetry yields the Lindblad equation [6] for the time dependence of the density matrix (given here in Sec. VIII), which applies in some extended versions of quantum mechanics [7]. In that case, there is just one matrix T_r, which can be identified with minus the Hamiltonian of the system.

We will now see what can be learned from the multiplication rule (17) for general continuous groups, when $g = g(\epsilon n)$ and $\overline{g} = g(\epsilon\overline{n})$ are both near the identity. Equation (17) is automatically satisfied if either $g = \mathbf{I}$ or $\overline{g} = \mathbf{I}$, so the lowest-order nontrivial terms in Eq. (17) are of order ϵ^2. The resulting condition is a terrible mess, involving many coefficients that only reflect how group elements are parametrized. To focus only on physically interesting quantities, we will ignore everything but the part of Eq. (17) that is antisymmetric in n and $\overline{n}$, which must be satisfied separately from the rest. Equation (17) would be symmetric in n and $\overline{n}$ if it were not for the nonvanishing commutators of the matrices $u^{(i)}$ on the left side of the equation and of the group elements themselves on the right side. To calculate the latter terms, we may write

$$\begin{aligned}g(\epsilon n)g(\epsilon\overline{n}) &= g[\epsilon n + \epsilon\overline{n} + \epsilon^2 f(n,\overline{n}) + \cdots],\\ f^r &= \frac{1}{2}\sum_{st} C^r_{st} n^s \overline{n}^t,\end{aligned} \tag{31}$$

where $C^r_{st} = -C^r_{ts}$ are the structure constants of the group's Lie algebra, and the dots in Eq. (31) denote second-order terms that are symmetric in n and $\overline{n}$, as well as terms of higher order in ϵ. The antisymmetric part of the terms in Eq. (17) of order ϵ^2 now gives

$$\begin{aligned}&[n\cdot\tau,\overline{n}\cdot\tau]\otimes\mathbf{1} + \mathbf{1}\otimes[n\cdot\tau,\overline{n}\cdot\tau]^\dagger\\ &\quad + i\sum_\alpha \Delta^{(\alpha)}(\overline{n})\,[\tau\cdot n, u^{(\alpha)}(\overline{n})]\otimes u^{(\alpha)\dagger}(\overline{n}) - i\sum_\alpha \Delta^{(\alpha)}(\overline{n})\,u^{(\alpha)}(\overline{n})\otimes[\tau\cdot n, u^{(\alpha)}(\overline{n})]^\dagger\\ &\quad - i\sum_\alpha \Delta^{(\alpha)}(n)\,[\tau\cdot\overline{n}, u^{(\alpha)}(n)]\otimes u^{(\alpha)\dagger}(n) + i\sum_\alpha \Delta^{(\alpha)}(n)\,u^{(\alpha)}(n)\otimes[\tau\cdot\overline{n}, u^{(\alpha)}(n)]^\dagger\\ &\quad - \frac{1}{2}\sum_{\alpha\beta}\Delta^{(\alpha)}(n)\,\Delta^{(\beta)}(\overline{n})\,[u^{(\alpha)}(n), u^{(\beta)}(\overline{n})]\otimes\{u^{(\alpha)}(n), u^{(\beta)}(\overline{n})\}^\dagger\\ &\quad - \frac{1}{2}\sum_{\alpha\beta}\Delta^{(\alpha)}(n)\,\Delta^{(\beta)}(\overline{n})\,\{u^{(\alpha)}(n), u^{(\beta)}(\overline{n})\}\otimes[u^{(\alpha)}(n), u^{(\beta)}(\overline{n})]^\dagger\\ &= i\sum_{rst}\tau_r\,C^r_{st}n^s\overline{n}^t\otimes\mathbf{1} - i\mathbf{1}\otimes\sum_{rst}\tau^\dagger_r\,C^r_{st}n^s\overline{n}^t - \sum_{rst}\left[\frac{\partial}{\partial(n+\overline{n})^r}\sum_\alpha\Delta^{(\alpha)}(n+\overline{n})u^{(\alpha)}(n+\overline{n})\otimes u^{(\alpha)\dagger}(n+\overline{n})\right]_{n+\overline{n}=0} C^r_{st}n^s\overline{n}^t,\end{aligned} \tag{32}$$

where curly brackets denote an anticommutator.

Inspection of Eq. (28) shows that if all $\Delta^{(\alpha)}$ vanish, then $\delta_{\epsilon n}\rho = i\epsilon[n\cdot T,\rho]$. Further, Eqs. (26) and (27) show in this case that $\tau_r = T_r$. Equation (32) then shows also that in this case the Hermitian matrices T_r satisfy the commutation relations $[T_s, T_t] = i\sum_r C^r_{st}T_t$ of the symmetry group's Lie algebra. So, if all Δ_α were zero, the transformation of the density matrix would be the same as in ordinary quantum mechanics.

But, these familiar results do not hold if the density matrix transforms in a more general way, with nonvanishing values

for some $\Delta^{(\alpha)}$, in which case the terms in Eqs. (28), (26), and (32) with nonzero $\Delta^{(\alpha)}$ represent a departure from ordinary quantum mechanics. In ordinary quantum mechanics, the structure of the Hamiltonian and other operators representing symmetry generators is largely fixed by the condition that they satisfy the Lie algebra of the symmetry group, as for instance the form of the kinetic energy terms in the nonrelativistic Hamiltonian is fixed by the commutators of the generator of time translation with the other generators of the Galilean group. In the generalization of quantum mechanics considered here, it is Eqs. (32) and (27) that must be used to constrain the operators T_r and $u^{(\alpha)}(n)$ that define the transformation of the density matrix.

V. AN EXAMPLE

The condition (32) sets constraints on the sorts of matrices T_r and $u^{(\alpha)}(n)$ that can enter in the transformation (28) of the density matrix for a given set of structure constants C^t_{rs}. This section will give an explicit example showing how these constraints can be satisfied, in a way different from that of ordinary quantum mechanics.

We will consider a group containing (perhaps among other things) two commuting symmetry operations, characterized by vectors n^r and $\overline{n}^r$ in the space of group parameters, for which $\sum_{rs} n^r \overline{n}^s C^t_{rs} = 0$. (One of these symmetry operations may be time translation.) To satisfy the constraints, let us try the assumption that the matrices $n \cdot T$, $\overline{n} \cdot T$, and the relevant $u^{(\alpha)}(n)$, $u^{(\alpha)\dagger}(n)$, $u^{(\beta)}(\overline{n})$, and $u^{(\beta)\dagger}(\overline{n})$ all here commute with one another [where by relevant we mean that $\Delta^{(\alpha)}(n)$ and $\Delta^{(\beta)}(\overline{n})$ are not all zero]. Then, the definition (26) and (27) shows that the matrices $n \cdot \tau$ and $\overline{n} \cdot \tau$ commute with each other and with the relevant $u^{(\alpha)}(n)$, $u^{(\alpha)\dagger}(n)$, $u^{(\beta)}(\overline{n})$, and $u^{(\beta)\dagger}(\overline{n})$. The constraint (32) is then satisfied, as every term in this constraint simply vanishes.

As simple as this example is, it represents a nontrivial generalization of ordinary quantum mechanics. Since the Hermitian $n \cdot T$ and the relevant $u^{(\alpha)}(n)$ and $u^{(\alpha)\dagger}(n)$ all here commute with one another, we can choose a basis in which they are all diagonal, with

$$[u^{(\alpha)}(n)]_{MN} = \delta_{MN}\, u_{\alpha M}(n), \quad [n \cdot T]_{MN} = \delta_{MN}\, n \cdot T_M.$$

The transformation (28) then reads as

$$[\delta_{\epsilon n}\rho]_{MN} = \epsilon \left\{ i n \cdot (T_M - T_N) + \sum_\alpha \Delta^{(\alpha)}(n) \left[u_{\alpha M}(n)\, u_{\alpha N}(n)^* - \frac{1}{2}|u_{\alpha M}(n)|^2 - \frac{1}{2}|u_{\alpha N}(n)|^2 \right] \right\} \rho_{MN},$$

so that ρ_{MN} is not simply multiplied by a difference $f(M) - f(N)$ for some function f, as in ordinary quantum mechanics. In the absence of any other symmetries, the parameters $\Delta^{(\alpha)}(n)$, $n \cdot T_M$, and $u_{\alpha M}(n)$ would be unconstrained, except that $\Delta^{(\alpha)}(n)$ and T_M are real.

VI. COMPACT GROUPS

A well-known theorem tells us that with a suitable choice of basis, all finite-dimensional representations of compact groups are unitary. The density matrix furnishes a d^2-dimensional representation of any symmetry group, so for compact groups it should transform unitarily. As we will now see, this does *not* mean that it undergoes the transformation $\rho \mapsto U\rho U^\dagger$ of ordinary quantum mechanics, but it does constrain its transformation properties in interesting ways, one of which will be important in dealing with the issue of positivity.

The unitarity of the transformation (3) requires that

$$\sum_{M''N''} K_{MM'',NN''}[g]\, K^*_{M'M'',N'N''}[g] = \sum_{M''N''} K^*_{M''M',N''N'}[g]\, K_{M''M,N''N}[g] = \delta_{M'M}\delta_{N'N}. \quad (33)$$

One immediate consequence that we will need in Sec. VII is that the density matrix $\rho = 1/d$ is invariant. We can see this by contracting the first equation (33) with δ_{MN} and using the trace condition Eq. (5). This gives

$$\sum_{M''} K^*_{M'M'',N'M''}[g] = \delta_{M'N'}.$$

Taking the complex conjugate and dividing by d then gives the statement of invariance:

$$g(\mathbf{1}/d) = \mathbf{1}/d. \quad (34)$$

In the notation (18), Eq. (33) reads as

$$\mathbf{1} \otimes \mathbf{1} = \sum_{ij} \eta^{(i)}[g]\eta^{(j)}[g] u^{(i)}[g] u^{(j)\dagger}[g] \otimes u^{(j)}[g] u^{(i)\dagger}[g] = \sum_{ij} \eta^{(i)}[g]\eta^{(j)}[g] u^{(i)\dagger}[g] u^{(j)}[g] \otimes u^{(j)\dagger}[g] u^{(i)}[g]. \quad (35)$$

For elements of continuous groups with parameters ϵn^r near the origin, we use Eqs. (23), (24), and (27) in Eq. (35), and find that

$$n \cdot \theta \otimes \mathbf{1} + \mathbf{1} \otimes n \cdot \theta = \sum_\alpha \Delta^{(\alpha)}[n]\, u^{(\alpha)}(n) \otimes u^{(\alpha)\dagger}(n) + \sum_\alpha \Delta^{(\alpha)}[n]\, u^{(\alpha)\dagger}(n) \otimes u^{(\alpha)}(n). \quad (36)$$

Taking the trace of the matrices on the right of the direct products then gives

$$d\, n \cdot \theta + \mathbf{1}\, \mathrm{Tr}(n \cdot \theta) = 0.$$

The trace of this equation gives $2d\, \mathrm{Tr}(n \cdot \theta) = 0$, so $n \cdot \theta = 0$, and therefore for compact groups

$$\tau_r = T_r. \quad (37)$$

VII. POSITIVITY

Finally, we come to the issue of positivity. It is clearly necessary that the linear mapping (3) corresponding to a symmetry transformation should take the density matrices of physical states into other density matrices that are positive as well as being Hermitian and having unit trace. A linear mapping is itself called *positive* if takes *all* positive Hermitian matrices into positive Hermitian matrices with the same trace. It would simplify matters if we could just assume that all symmetry mappings are positive, but this is not indispensable

because the density matrices of physical states may be limited in some way that ensures that they are mapped into positive matrices, even if some other positive matrices are not mapped into positive matrices [13].

The existence of constraints on physical density matrices that ensure that they transform into other positive density matrices is particularly plausible for compact symmetry groups, for which for any ρ, $g(\rho)$ varies only over a compact manifold. For instance, in the SU(3) example of Sec. I, the density matrix is positive if (though not only if) all diagonal elements a_i are positive and the off-diagonal elements b_i are subject to the inequality

$$|b_1|^2 + |b_2|^2 + |b_3|^2 \leqslant \tfrac{1}{4} a_1 a_2 a_3.$$

This condition is SU(3) invariant, so under SU(3) transformations any density matrix satisfying this condition will be transformed into another density matrix satisfying the same condition, and will therefore also be positive.

This is an important point because, as we shall now show. if the mapping associated with any invertible continuous symmetry acts on *all* density matrices as a positive mapping, then this mapping must take the same form (2) as in ordinary quantum mechanics. For the purposes of this theorem, we only need to show that for any invertible mapping that is not of the form (2) there is *some* positive density matrix ρ that is transformed into a nonpositive matrix, so we are free to choose ρ here pretty much as we like. We will choose the density matrix ρ to have one eigenvector v with eigenvalue zero:

$$\rho v = v^\dagger \rho = 0. \tag{38}$$

When we take the expectation value of Eq. (28) in the "state" v, as a consequence of Eq. (38) we find that only the first term in the quantity summed over α makes a nonzero contribution:

$$\begin{aligned}(v^\dagger [\rho + \delta_{\epsilon n}\rho] v) &= (v^\dagger\, \delta_{\epsilon n}\rho\, v\,) \\ &= \epsilon \sum_\alpha \Delta^{(\alpha)}(n)\, [v^\dagger u^{(\alpha)}(n)\, \rho\, u^{(\alpha)\dagger}(n) v]. \end{aligned} \tag{39}$$

It is immediately obvious that if the coefficient of ϵ is nonzero, then for some sign of ϵ the expectation value (39) will be negative, so that $\rho + \delta_{\epsilon n}\rho$ cannot be positive.

It only remains to show that unless all $\Delta^{(\alpha)}(n)$ vanish, for some vector v there will be some positive Hermitian matrix ρ satisfying Eq. (38) for which the coefficient of ϵ in Eq. (39) is nonzero. [This is obvious if all $\Delta^{(\alpha)}(n)$ have the same sign, but we want also to consider the case where some are positive and some are negative.] Let us suppose the contrary; that is, for some n and for all v we have

$$\sum_\alpha \Delta^{(\alpha)}(n)\, [v^\dagger u^{(\alpha)}(n)\, \rho\, u^{(\alpha)\dagger}(n) v] = 0 \tag{40}$$

for all positive Hermitian matrices ρ satisfying Eq. (38). We will show that in this case, we must have $\Delta^{(\alpha)}(n) = 0$ for all α.

We are free to take ρ to have no eigenvectors with eigenvalue zero other than v. In this case, the condition that ρ is positive puts no constraints on infinitesimal variations of ρ, so the assumption that Eq. (40) holds for all positive Hermitian ρ satisfying Eq. (38) requires that

$$\sum_\alpha \Delta^{(\alpha)}(n)\, [v^\dagger u^{(\alpha)}(n)]_M\, [u^{(\alpha)\dagger}(n) v]_N = c_M^* v_N + v_M^* c_N \tag{41}$$

for all N and M, and for some vector c_N which may depend on n and v. In fact, c_N must depend on v because Eq. (41) is supposed to hold for all v, so there have to be the same numbers of v's and v^*'s on both sides of the equation. Specifically, we must have $c_N = \sum_L C_{NL} v_L$, where C_{NL} is independent of v, and the coefficient of $v_P^* v_Q$ in Eq. (41) must vanish:

$$\sum_\alpha \Delta^{(\alpha)}(n)\, u^{(\alpha)}_{PM}(n)\, u^{(\alpha)\dagger}_{NQ}(n) = C^*_{MP}\delta_{NQ} + \delta_{MP} C_{NQ}. \tag{42}$$

Now, we can use some of the properties of the $u^{(\alpha)}(n)$ obtained in Sec. IV. Consider any β, and contract Eq. (42) with $u^{(\beta)\dagger}_{MP}(n) u^{(\beta)}_{QN}(n)$. Because the $u^{(\beta)}(n)$ are traceless, the right-hand side of the contracted equation vanishes, and because they satisfy the orthonormality condition $\mathrm{Tr}(u^{(\beta)\dagger} u^{(\alpha)}) = \delta_{\beta\alpha}$, the left-hand side of the contracted equation is $\Delta^{(\beta)}(n)$, so $\Delta^{(\beta)}(n) = 0$ for all β, as was to be shown.

This theorem leaves open the possibility of limiting the density matrix to a special class of positive Hermitian matrices, for which any symmetry transformation takes any member of this class into another positive member of the same class, as in the SU(3) example given above. But, does such a special class always exist? A hand-waving argument suggests that it does, at least for compact groups. We saw in the previous section that in a suitable basis, such symmetries leave invariant the positive density matrix $1/d$. Suppose we shift this density matrix by some traceless Hermitian matrix η. The new density matrix $1/d + \eta$ will generally not be invariant, but as long as η is sufficiently small, the symmetry transformations belonging to a compact group will take $1/d + \eta$ into density matrices whose eigenvalues are all sufficiently close to the original common eigenvalue $1/d$ so that they are still all positive. Thus, acting on a density matrix $1/d + \eta$ with all symmetries g belonging to a compact group, and with η running over all traceless Hermitian matrices that are sufficiently small so that all $g(1/d + \eta)$ are positive, provides the sort of special class of density matrices we need, which can transform in a way that is different from the transformation (2) of ordinary quantum mechanics without raising problems with positivity.

VIII. MAPPINGS WITH POSITIVE EIGENVALUES

There is a class of mappings that are obviously positive, in the sense of taking all positive Hermitian matrices into positive Hermitian matrices. Inspection of Eq. (13) shows immediately that a mapping is positive if (though not only if) all its eigenvalues $\eta^{(i)}$ are positive. In this case, we can write the general mapping (13) in the Kraus form [14]:

$$g(\rho) = \sum_i \mathcal{U}^{(i)}[g]\, \rho\, \mathcal{U}^{(i)\dagger}[g], \tag{43}$$

where $\mathcal{U}^{(i)}[g] \equiv \eta^{(i)}[g]^{1/2} u^{(i)}[g]$ and $\sum_i \mathcal{U}^{(i)\dagger}[g]\mathcal{U}^{(i)}[g] = 1$. The unitary transformations $\rho \mapsto U[g]\, \rho\, U[g]^\dagger$ of ordinary quantum mechanics are a special case of the more general

transformations (43), distinguished by the sum in (43) having just a single term.

The assumption that all eigenvalues of the kernel are positive would be an effective way of guaranteeing that all positive density matrices are mapped into positive density matrices, but it would have the consequence that the transformation of the density matrix under any symmetry group, whether continuous or discrete, would reduce to the same unitary transformation rule (2) as in ordinary quantum mechanics.

We can see this immediately for continuous groups. If for some infinitesimal continuous symmetry transformation $g[\epsilon n]$ we were to require the positivity of the eigenvalues (23) whatever the sign of ϵ, we would have to assume that $\Delta^{(\alpha)}(n) = 0$ for all α. As already mentioned in Sec. IV, any continuous symmetry for which $\Delta^{(\alpha)}(n)$ vanishes for all α is necessarily realized by the unitary transformation (2) of ordinary quantum mechanics. Of course, we already knew this. With all eigenvalues positive, mappings preserve the positivity of *any* density matrix, and as shown in the previous section, any invertible continuous symmetry that preserves the positivity of all density matrices must act as in Eq. (2).

As already mentioned in Sec. I, in various extended versions of quantum mechanics [7] the assumption of positive mapping of the density matrix is commonly made for the continuous symmetry of time translation, but only prospectively, not retrospectively. It is usually assumed in these theories that the kernel for time translation by an amount τ has positive eigenvalues if $\tau > 0$, but this is not assumed (and in fact is not generally true) when $\tau < 0$. For this reason, the positive time-translation mappings usually considered in these theories form a semigroup, not a group. With this weaker assumption, Eq. (23) simply requires that $\Delta^{(\alpha)}(n_{\mathcal{T}}) \geqslant 0$ for all α, where $n_{\mathcal{T}}$ denotes the direction in the space of group parameters for time translation. The transformation rule (28) then immediately yields the Lindblad equation

$$\frac{d}{dt}\rho = -i[H,\rho] + \sum_{\alpha}\left[L_\alpha\,\rho\,L_\alpha^\dagger - \frac{1}{2}L_\alpha^\dagger\,L_\alpha\,\rho - \frac{1}{2}\rho\,L_\alpha^\dagger\,L_\alpha\right],$$

where $H \equiv -n_{\mathcal{T}}\cdot T$ and $L_\alpha \equiv \Delta^{(\alpha)1/2}(n_{\mathcal{T}})\,u^{(\alpha)}(n_{\mathcal{T}})$. This implies that the observable represented by an operator A is conserved, in the sense that $\overline{A} = \mathrm{Tr}(A\rho)$ is time independent for all ρ, if

$$0 = i[H,A] - \sum_{\alpha}\left[L_\alpha^\dagger\,A\,L_\alpha - \frac{1}{2}L_\alpha^\dagger\,L_\alpha\,A - \frac{1}{2}A\,L_\alpha^\dagger\,L_\alpha\right].$$

Unfortunately, for the general symmetry transformations considered here, there does not seem to be any connection between such conserved quantities and the generators of symmetries.

If $\rho(t)$ is positive for some initial time t, then the Lindblad equation gives a positive $\rho(t')$ for all $t' > t$ but, as illustrated in Ref. [8], in these theories one can usually find an earlier time $t' < t$ for which $\rho(t')$ is not positive. As I understand it, this is tolerated in extended versions of quantum mechanics in which the Lindblad equation is applied to closed systems because unless we tackle the description of the whole universe, the differential equation for the time dependence of the density matrix is only supposed in these theories to apply for systems that become closed at some initial time t, so one does not have to worry about what happens for times $t' < t$.

One can argue about whether this is satisfactory for time translation, but we would certainly not want to assume that the eigenvalues of $K[g]$ are all positive when the symmetry transformation g is a spatial translation to the north but not to the south, or is a rotation that is clockwise around the vertical but not counterclockwise, or is a boost that increases the velocity to the eastward but not to the westward. Such symmetry transformations must be assumed to form a group, not merely a semigroup.

With a little more effort, we can show that for all symmetry groups, discrete as well as continuous, the assumption of positive eigenvalues rules out the possibility that the density matrix will have an unusual transformation rule, one different from Eq. (2). To prove this, we use one of the defining properties of groups, that for every element g of a group there is an inverse g^{-1}. From Eq. (16) and Eqs. (19)–(21), with $\overline{g}$ taken as g^{-1}, we have

$$\sum_{ij}\eta^{(i)}[g]\,\eta^{(j)}[g^{-1}]\,u^{(i)}[g]\,u^{(j)}[g^{-1}]\,\rho\,u^{(j)\dagger}[g^{-1}]\,u^{(i)\dagger}[g] = \rho \tag{44}$$

for any matrix ρ. In particular, for a Hermitian matrix ρ, we can find a unitary matrix Ω such that $\rho^{(\mathrm{D})} = \Omega\rho\Omega^{-1}$ is diagonal, $[\rho^{(\mathrm{D})}]_{MN} = P_M\delta_{MN}$. Equation (44) then applies if we replace ρ with $\rho^{(D)}$ and replace all $u^{(i)}[g]$ and $u^{(j)}[g^{-1}]$ with $u^{(i\mathrm{D})}[g] \equiv \Omega u^{(i)}[g]\Omega^{-1}$ and $u^{(j\mathrm{D})}[g^{-1}] \equiv \Omega u^{(j)}[g^{-1}]\Omega^{-1}$. This gives

$$\sum_{ij}\eta^{(i)}[g]\,\eta^{(j)}[g^{-1}]\sum_{L}\left[u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]\right]_{ML} \times P_L\left[u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]\right]^*_{NL} = P_M\delta_{MN}. \tag{45}$$

This must hold for all real numbers P_N, so it follows that, for all L, M, and N,

$$\sum_{ij}\eta^{(i)}[g]\,\eta^{(j)}\left[g^{-1}\right]\left[u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]\right]_{ML} \times\left[u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]\right]^*_{NL} = \delta_{ML}\delta_{NL}. \tag{46}$$

In particular, if $M = N \neq L$, then

$$\sum_{ij}\eta^{(i)}[g]\,\eta^{(j)}[g^{-1}]\,\left|\left[u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]\right]_{ML}\right|^2 = 0. \tag{47}$$

Here is where the positivity of the eigenvalues becomes important. If all the eigenvalues $\eta^{(i)}[g]$ and $\eta^{(j)}[g^{-1}]$ are positive, then it follows from Eq. (47) that for all relevant i and j (that is, for all i and j for which $\eta^{(i)}[g]$ and $\eta^{(j)}[g^{-1}]$, respectively, do not vanish) we have

$$\left[u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]\right]_{ML} = 0 \tag{48}$$

for any unequal indices M and L. Since the matrix $u^{(i\mathrm{D})}[g]\,u^{(j\mathrm{D})}[g^{-1}]$ is thus diagonal, it commutes with the diagonal matrix $\rho^{(\mathrm{D})}$. But then also $u^{(i)}[g]\,u^{(j)}[g^{-1}]$ commutes with the arbitrary Hermitian matrix ρ. The only matrices that commute with all Hermitian matrices are proportional to the unit matrix, so we can conclude that for all relevant i and j

$$u^{(i)}[g]\,u^{(j)}[g^{-1}] = c_{ij}[g]\mathbf{1} \tag{49}$$

for some complex numerical coefficients $c_{ij}[g]$. Taking the determinant of Eq. (49) gives $(c_{ij}[g])^d = \mathrm{Det}u^{(i)}[g]\,\mathrm{Det}u^{(j)}[g^{-1}]$. Now, there must be at least one relevant j

for which $\mathrm{Det}u^{(j)}[g^{-1}] \neq 0$ since otherwise we would have $u^{(i)}[g]\,u^{(j)}[g^{-1}] = 0$ for all relevant i and j, contradicting Eq. (44). Taking j to have any value for which $\mathrm{Det}u^{(j)}[g^{-1}] \neq 0$, Eq. (49) then tells us that all relevant $u^{(i)}[g]$ are proportional to a single $u[g]$; specifically,

$$u^{(i)}[g] = \left(\mathrm{Det}u^{(i)}[g]\right)^{1/d} u[g], \tag{50}$$

where $u[g] = u^{(j)-1}[g^{-1}](\mathrm{Det}u^{(j)}[g^{-1}])^{1/d}$. The trace condition (14) then reads as

$$\sum_i \eta^{(i)}[g]\,\left|\mathrm{Det}u^{(i)}[g]\right|^{2/d} u^\dagger[g]u[g] = 1,$$

so the matrix $U[g] \equiv [\sum_i \eta^{(i)}[g]\,|\mathrm{Det}u^{(i)}[g]|^{2/d}]^{1/2}u[g]$ is unitary, and the transformation rule (13) takes the familiar form $g(\rho) = U[g]\,\rho\,U^\dagger[g]$ of ordinary quantum mechanics, as was to be proved.

But, do we need to require that the kernels for general symmetries have only positive eigenvalues? There are well-known examples of positive mappings that have some negative eigenvalues. The standard example is the transposition map

$$K_{M'M,N'N} = \delta_{M'N}\delta_{N'M}.$$

This has two eigenvalues, one positive and one negative. (Any symmetric or antisymmetric matrix is an eigenmatrix with eigenvalue $+1$ or -1, respectively.) Nevertheless, K is positive because $g(\rho) = \rho^{\mathrm{T}}$, which is positive if ρ is positive.

There is a widely cited argument for the requirement that all eigenvalues of the kernel K must be positive, based on the possibility of entanglement. Consider an arbitrary system $\mathcal{S}^{(I)}$, and an arbitrary linear mapping $K^{(I)}$ of the density matrix of this system, which preserves its Hermiticity, unit trace, and positivity. We can imagine adding an isolated system $\mathcal{S}^{(II)}$ of finite dimensionality d_{II}, and extending $K^{(I)}$ to a kernel K that acts as $K^{(I)}$ on $\mathcal{S}^{(I)}$, and acts trivially on $\mathcal{S}^{(II)}$. That is, if we label the basis vectors of $\mathcal{S}^{(I)}$ with indices m, n, etc. and the basis vectors of $\mathcal{S}^{(II)}$ with indices a, b, etc., the kernel of the mapping [in the notation of Eqs. (3) and (6)] on the combined system is

$$K_{m'a'ma,n'b'nb} = K^{(I)}_{m'm,n'n}\delta_{a'a}\delta_{b'b}. \tag{51}$$

The original mapping $K^{(I)}$ is said to be *completely positive* [15] if K is positive (in the sense of mapping all positive density matrices for the combined system into positive density matrices) for all finite dimensionalities d_{II}. A theorem due to Choi [16] states that if $K^{(I)}$ is completely positive in this sense, then all its eigenvalues are positive. [As usually stated, the theorem says that any completely positive mapping takes the Kraus form (43), but as we have seen this form follows from the positivity of the eigenvalues, and it is obvious that any kernel that induces a transformation of this form has only positive eigenvalues, so the two statements of the theorem are equivalent.]

Although there is no doubt of the mathematical correctness of the Choi theorem, it is not clear that it is relevant physically. It should be noted that the vacuum is the only physical system that is invariant under Galilean (or Lorentz) transformations and time translations. Since the dimensionality of the Hilbert space of the vacuum is unity, this does not fulfill the conditions of the Choi theorem, that there should be isolated systems $\mathcal{S}^{(II)}$ with arbitrary finite dimensionality on which the symmetry acts trivially. There seems to be a widespread impression that this does not matter, at least for the only symmetry that has been previously studied in this context, the symmetry of time translation. It is supposed that, even if a symmetry transformation K acts nontrivially on $\mathcal{S}^{(II)}$, we may be able to undo it by inventing a transformation L that acts on $\mathcal{S}^{(II)}$ as the inverse of K, and leaves $\mathcal{S}^{(I)}$ unchanged, so that LK does have the form (51). (I have not been able to find a published reference to this argument.) But, in general, except in the uninteresting case in which $\mathcal{S}^{(I)}$ is the vacuum, L will not be a symmetry transformation, so neither will be LK. Or, if we take L as a symmetry transformation that acts nontrivially on $\mathcal{S}^I$, then the action of LK on the Hilbert space of $\mathcal{S}^I$ is a completely positive mapping, but it is not the same mapping as $K^{(I)}$. There are some continuous symmetry transformations, such as rotations, for which there are invariant physical systems with Hilbert spaces of arbitrary dimensionality which therefore might be taken as the isolated system $\mathcal{S}^{(II)}$ in the assumptions of the Choi theorem. Even so, in the real world there are no disembodied spins, only particles with spins. The Hilbert space of any physical system other than the vacuum has infinite dimensionality, and it is not clear that the Choi theorem can be extended to realistic cases.

Even though it may be doubted whether complete positivity in the sense of Choi is physically necessary, there is another requirement that does seem to be inescapably necessary, and that leads to the same conclusion about positive eigenvalues. If some system $\mathcal{S}$ is physically realizable, then the system $\mathcal{S}\otimes\mathcal{S}$ consisting of two isolated copies of $\mathcal{S}$ will presumably also be realizable. Any symmetry that acts on the density matrix of $\mathcal{S}$ with a kernel K will act on the density matrix of the combined system with a kernel given by a direct product $K\otimes K$, as in Eq. (6), with $K^{(I)} = K^{(II)} = K$. Benatti, Floreanini, and Romano [17] have shown that, in this case, in order for $K\otimes K$ to be positive (in the sense of transforming all entangled positive Hermitian density matrices for $\mathcal{S}\otimes\mathcal{S}$ into positive Hermitian density matrices) it is necessary not only that K be positive, but also completely positive, so that all eigenvalues of K are positive.

This might seem to rule out any transformation rules for the density matrix different from those of ordinary quantum mechanics. But, we have already seen in Sec. VII that it is necessary to limit physically allowable density matrices in order to maintain their positivity under continuous symmetry group transformations different from those of ordinary quantum mechanics. Similarly, we may have to restrict the allowed density matrices in a way that rules out the density matrices for combined systems $\mathcal{S}\otimes\mathcal{S}$ that are considered in the theorem of Benatti *et al.*

Despite these skeptical comments, it may turn out to be physically necessary for the kernels $K[g]$ for all elements g of symmetry transformation groups to have only positive eigenvalues. In that case, the main point of this paper would be the proof that such symmetry transformations act on the density matrix as in ordinary quantum mechanics. It would be much more interesting if for some symmetry groups it will turn out to be unnecessary for all eigenvalues to be positive, in which case the much richer variety of symmetry transformations discussed in Secs. II and III would be physically possible.

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