Foundations of Physics, Vol. 9, Nos. 7/8, 1979

Superselection Rules in Quantum Theory: Part I. A New Proposal for State Restriction Violation

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Received June 15, 1978

It is argued that preparation of a quantum state characterized by density operator ρ *not commuting with a superselection operator* Q *does not by itself constitute an instance of superselection rule violation. It would, however, be an instance of state restriction violation. It is held that superselection rule violation is only possible with simultaneous observable and state restriction violations. It is shown that it is a priori conceivable to subdivide an ensemble whose* ρ *satisfies* $[\rho, Q] = 0$ *into subensembles whose density operators violate the state restrictions. The dynamics of the subdivision process is not considered.*

1. INTRODUCTION

Superselection rules were first introduced to quantum theory in a brief paper published in 1952 by Wick, Wightman, and Wigner (WWW).[1] We may paraphrase their fundamental postulate as follows:

Postulate P (Superselection Rule Postulate). The Hilbert space H is decomposable into a direct sum of orthogonal subspaces H_q such that the relative phases of the components in different subspaces H_q of any state vector are intrinsically irrelevant.

If P is satisfied there exists a *superselection operator* Q whose eigenspaces are the subspaces H_q (the generic term "charge" is not necessarily the electric charge). We denote the spectral family of Q by P_q, i.e., P_q is the projection for the H_q eigenspace associated with Q eigenvalue q. Since H_q is in general multidimensional, we write

$$P_q = \sum_{d_q} P_{qd_q} \tag{1}$$

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0015-9018/79/0800-0537$03.00/0

where P_{qd_q} is a one-dimensional projection operator; d_q is a degeneracy index for the Q eigenvalue q.

To derive a mathematical condition equivalent to P, let ψ and ψ' be arbitrary state vectors defined as

$$\psi = \sum_q P_q \psi = \sum_{qd_q} P_{qd_q} \psi \equiv \sum_{qd_q} \psi_{qd_q} \mid qd_q \rangle \tag{2}$$

and

$$\psi' = \sum_{qd_q} e^{i\alpha_q} \psi_{qd_q} \mid qd_q \rangle \tag{3}$$

where the α_q are real constants, $\mid qd_q \rangle$ are the Q eigenvectors, and the components ψ_{qd_q} are arbitrary. P asserts that all the α_q are "intrinsically irrelevant." In common parlance this is taken to mean that ψ and ψ' are equivalent in the sense that the measurement statistics of two homogeneous ensembles, one characterized by ψ and the other by ψ', are identical. Mathematically, this is expressed as

$$\mathrm{Tr}(P_{\psi'} A) - \mathrm{Tr}(P_\psi A) = 0 \tag{4}$$

where A is any observable. Therefore

$$\sum_{qd_q q' d'_{q'}} \{\exp[i(\alpha_q - \alpha_{q'})] - 1\} \, \psi_{qd_q} \psi^*_{q'd'_{q'}} A_{q'd'_{q'};qd_q} = 0 \tag{5}$$

where

$$A_{q'd'_{q'};qd_q} \equiv \langle q'd'_{q'} \mid A \mid qd_q \rangle \tag{6}$$

Equation (5) is the mathematical counterpart to P, valid for any state vector ψ and any observable A.

It is not difficult to write down two separate sufficient conditions for (5):

Proposition S (State Restrictions). For any state vector ψ,

$$\psi_{qd_q} \psi^*_{q'd'_{q'}} = \delta_{qq'} \psi_{qd_q} \psi^*_{qd'_q} \tag{7}$$

Proposition O (Observable Restrictions). For any observable A,

$$A_{q'd'_{q'};qd_q} = \delta_{qq'} A_{qd'_q;qd_q} \tag{8}$$

The state restrictions S amount to a limitation on the general validity of the superposition principle: any state vector must be a charge eigenvector if S is satisfied. The observable restrictions O imply that not all Hermitian operators correspond to observables; note that

$$[A, Q]_{q'd'_{q'};qd_q} = (q - q')\, A_{q'd'_{q'};qd_q} \tag{9}$$

so that A commutes with Q if O is satisfied.

Both S and O are usually taken as necessarily true if P is true. Inspection of (5) shows that this position is stronger than required; apparently particular ψ and A could conspire to satisfy (5) even though neither S nor O was satisfied. It is therefore somewhat surprising that the hallmark of superselection rules is usually taken to be the validity of S *and* O. This view is attributable to an uncritical adoption of the projection postulate, according to which the measurement of an observable A is accompanied by reduction of the quantum state to an eigenstate of A belonging to the measured eigenvalue. Such an axiom confounds the distinction between state preparation and measurement and, among other dubious consequences, does indeed imply an equivalence between S and O. However, since we do not accept the projection postulate,[2] the present investigation does not presuppose that S and O are equivalent.

Just what then is the logical status of S and O in relation to P? We answer this question by studying the logical relationships between S and O. Let $\sim O$ denote the negation of O; we begin by assuming $\sim O$. Thus (5) should hold for $A = P_\psi$ and hence

$$A_{q'd'_{q'};qd_q} = \psi_{q'd'_{q'}} \psi^*_{qd_q} \tag{10}$$

When this is substituted in (5) we find

$$\sum_{qd_q q'd'_{q'}} [\cos(\alpha_q - \alpha_{q'}) - 1]\, |\, \psi_{qd_q} \psi_{q'd'_{q'}} |^2 = 0 \tag{11}$$

Since the phases are irrelevant, this result should be invariant with respect to changes in the α_q, for any ψ. Therefore, the components ψ_{qd_q} satisfy S, and we have shown that if P is true, then $\sim O \Rightarrow S$. Therefore

$$P \Rightarrow S \vee O \tag{12}$$

where $\vee$ denotes logical disjunction ("or"). Of course, we know that either S or O alone implies P. Therefore

$$P \Leftrightarrow S \vee O \tag{13}$$

However, we must take issue with the usual assertion,

$$P \Leftrightarrow S \wedge O \tag{14}$$

where $\wedge$ denotes logical conjunction ("and"). The above analysis indicates that $S \wedge O$ is too strong; there might, for instance, exist situations of the type $P \wedge \sim O$.

The logical status of S and O has considerable influence on how one might propose to violate a superselection rule. Obviously, if (14) is true then one need only prepare an *illegal* state, i.e., one violating S. All of the previously proposed schemes for violation of superselection rules fall into this category. There are no published attempts to violate superselection rules by violating S and O simultaneously, the only consistent way to do this. Part I of this work establishes the mathematical possibility of state restriction (S) violation by considering alternative decompositions of density operators. Part II then goes on to consider the ensemble subdivision problem in a superselection rule context and the possibility of superselection rule violation by simultaneous S and O violation employing a correlation scheme.

2. EXTANT THEORIES OF SUPERSELECTION RULES

This section reviews the two most common formulations of superselection rules, noting the logical status of the state and observable restrictions in each. These are due to WWW and Bogolubov, Logunov, and Todorov (BLT).[4]

The original 1952 superselection rule paper by WWW asserted the nonmeasurability of an observable whose operator correspondent does not commute with the superselection operator.[1] They therefore argued that not all Hermitian operators correspond to observables: their 1952 paper insists on Proposition O (cf. Section 1). We do not understand this position of WWW: we would agree that measurement of an observable not commuting with Q is in all likelihood equivalent to measurement of an observable commuting with charge, but that is not to say that O necessarily holds. We prefer to interpret the WWW formalism in our more liberal sense, as outlined in Section 1, which does not *necessarily* require O.

In 1970 WWW published another paper on superselection rules.[3] This paper included a generalization of the state restriction Proposition S (cf. Section 1) to the general case of a mixed quantum state. We will outline their reasoning to the generalization S' of S.

Proposition S′ (State Restrictions). For any quantum state ρ,

$$\rho_{q'd'_{q'};qd_q} = \delta_{qq'}\rho_{qd'_q;qd_q} \tag{15}$$

The validity of S' of course entails that ρ commutes with Q. A density operator meeting this condition is said to be *compatible* with the superselection rule, *permissible*, or, as we sometimes like to say, *legal*. The corresponding ensemble will also be designated as compatible, permissible, or legal.

We begin by stating that the state vector

$$\psi = \sum_{qd_q} \psi_{qd_q} \mid qd_q\rangle \tag{16}$$

is *legal* if the components ψ_{qd_q} satisfy

$$\psi_{qd_q} = \delta_{qq_0}\psi_{d_q} \tag{17}$$

with q_0 fixed. Such a ψ satisfies S and has nonvanishing components in only one Q eigenspace H_q. If an ensemble is characterized by a state vector ψ, the corresponding density operator is (ψ normalized)

$$\rho = P_\psi \tag{18}$$

If ψ is legal, then WWW assume that this ρ is also. Then WWW arrive at the general form of a permissible density operator with the following premiss:

Premiss W. The most general permissible ensemble is a mixture of subensembles each of which is characterized by a legal state vector.

In other words, the most general permissible ensemble is a mixture of permissible *homogeneous* subensembles.

Before continuing with the derivation of the permissible form we would like to mention that W is more an operational definition than a mathematical fact. This is easily shown by considering the spectral expansion of any density operator,

$$\rho = \sum_k w_k P(w_k) \tag{19}$$

Here the w_k are ρ eigenvalues and the $P(w_k)$ are the projections onto the w_k eigenspaces. Since these eigenspaces are multidimensional if ρ has a degenerate spectrum, the $P(w_k)$ are not necessarily one-dimensional projections. If Q commutes with ρ, it commutes with any function of ρ, hence with any $P(w_k)$. Each $P(w_k)$ can be decomposed as

$$P(w_k) = \sum_{d_k} P_{\alpha_{kd_k}} \tag{20}$$

where α_{kd_k} is an eigenvector of ρ belonging to ρ eigenvalue w_k: the α_{kd_k} can be illegal with $P(w_k)$ still commuting with Q! Thus it is mathematically conceivable for a permissible ensemble to be a mixture of not necessarily permissible homogeneous subensembles. That is why we regard W as an operational definition.

Let us continue with the derivation of the genral permissibility criterion. According to W, ρ is permissible if

$$\rho = \sum_q w_q P_{\psi_q} \tag{21}$$

where

$$\psi_q = \Big(\sum_{d_q} \psi_{d_q} \mid qd_q\rangle\Big)\Big(\sum_{d_q} \mid \psi_{d_q} \mid^2\Big)^{-1/2} \tag{22}$$

and

$$\sum_q w_q = 1 \tag{23}$$

A simple calculation gives the result

$$\rho_{qd_q;q'd'_{q'}} = \delta_{qq'} w_q \psi_{d_q} \psi^*_{d'_{q'}} \Big/ \sum_{d_q} \mid \psi_{d_q} \mid^2 \tag{24}$$

which is the block-diagonal Q-representation form given in (15). From

$$[\rho, Q]_{q'd'_{q'};qd_q} = (q - q')\, \rho_{q'd'_{q'};qd_q} \tag{25}$$

it is easy to see that commutativity of ρ with Q is both necessary and sufficient for the permissibility of ρ.

The genralized state restriction S' is a sufficient condition for the Superselection Rule Postulate P given in Section 1. To see this one considers the problem of measuring the relative phases of ψ, ψ' as given in (2) and (3) under the stipulation that any quantum state ρ obey S'. Measurability of the relative phases entails

$$\mathrm{Tr}[\rho(P_{\psi'} - P_\psi)] \neq 0 \tag{26}$$

for any quantum state ρ. A straightforward calculation shows that this requires

$$\sum_{qd_q q'd'_{q'}} \{\exp[i(\alpha_q - \alpha_{q'})] - 1\}\, \psi_{qd_q} \psi^*_{q'd'_{q'}} \rho_{q'd'_{q'};qd_q} \neq 0 \tag{27}$$

which cannot be met if (15) is satisfied. Therefore the WWW generalized permissibility criterion as expressed by Proposition S' is sufficient for the Superselection Rule Postulate P.

In summary, the state and observable restrictions in the WWW formulation are conveniently expressed by commutativity of the corresponding operators with a superselection operator. Obviously it is consistent with

WWW to demand only that those are sufficient conditions for the superselection rule to be in effect, i.e.,

$$P \Rightarrow S \vee O \tag{28}$$

BLT presented a concise axiomatic treatment of the foundations of superselection rules in their 1969 book on axiomatic quantum field theory, which first appeared in English translation in 1975.[4] We will only outline this formulation, with the aim of understanding the logical status of the restrictions on the observables and quantum states within its context.

The central theoretical notion of the BLT formulation is the concept of *coherence*, a topological property attributed to some subsets of H. A *coherent subset* of H is any subset of H which cannot be partitioned into mutually orthogonal nonempty subsets. More specifically, $M_\alpha \subseteq H$ is coherent if it is impossible to find orthogonal nonempty subsets $R_\alpha \subseteq H$ and $S_\alpha \subseteq H$ such that $M_\alpha = R_\alpha \cup S_\alpha$. This concept is used in two lemmas, stated here without proof.

Lemma (BLT). A necessary and sufficient condition for a subset $M \subseteq H$ to be coherent is that any bounded operator on its closed linear span $L(M)$ that commutes with all projections Π_ψ on M is a constant multiple of the identity on $L(M)$.

Lemma (BLT). Let M be a nonempty set of nonzero vectors in the Hilbert space H. Then $L(M)$ can be decomposed into a direct sum of orthogonal subspaces, $L(M) = \bigoplus_\alpha L_\alpha$, in such a way that each set $M_\alpha = M \cap L_\alpha$ is coherent and $M = \bigcup_\alpha M_\alpha$.

The first lemma gives a mathematical characterization of *coherence*. The projections Π_ψ are proportional to the operator $|\psi\rangle\langle\psi|$, where $|\psi\rangle \in M$. The second lemma shows that the closed linear span of any subset of H can be partitioned into coherent subspaces.

The BLT formalism was apparently designed with the idea in mind that not all elements of the Hilbert space H could represent pure quantum states; those that can are called *physical vectors* and correspond to those vectors in H that are legal, i.e., the possible state vectors. A fundamental postulate of their formulation is that the set M above is the set of physical vectors, i.e., it exhausts all possible state vectors, and the closure of M is H.

By definition, a BLT observable is any operator A satisfying the following conditions: (a) A is self-adjoint; (b) the domain D_A of A is dense in H; (c) $D_A \cap M$ is dense in M; (d) each M_α reduces A.

It follows then that the coherent subspaces M_α are the eigenspaces of any BLT superselection operator Q. Moreover, any BLT observable must commute with Q. The general matrix form of any observable is epitomized as a block-diagonal matrix in a representation whose basis vectors are the eigenvectors belonging to the distinct eigenvalues of Q. The eigenvectors of Q are physical vectors and conversely. The scheme for the preparation of any homogeneous ensemble is always characterized by a legal vector: state restrictions on pure states are unavoidable in the BLT formalism. If it is granted that the most general ensemble is a statistical mixture of homogeneous subensembles, the same state restrictions apply to the general BLT quantum state.

Therefore the WWW and BLT formulations of superselection rules differ in the logical status of the state and observable restrictions. The WWW version starts from a postulate concerning measurability of relative phases, with the result that both restrictions are individually sufficient but not necessary for the superselection rule. On the other hand, BLT start by assuming that the set of physical vectors M is a proper subset of the entire Hilbert space H, with the result that all observables and all states necessarily obey the restrictions.

3. PREVIOUS PROPOSALS FOR SUPERSELECTION RULE VIOLATION

Previous proposals for superselection rule violation[5–8] consist of arguments for the preparation of illegal quantum states. Apparently the authors of these proposals consider the state restrictions a necessary condition for the superselection rule. As we mentioned earlier, this logical status seems too strong to us, and thus we would not take these proposals as serious challenges unless accompanied by a simultaneous prescription for violation of the observable restrictions. However, even if the state restrictions are logically necessary, these proposals do not legitimately challenge the superselection rule, since they beg the question. This has been elegantly demonstrated by WWW.[3] All previous schemes for state restriction violation appear to require illegal quantum states initially.

This flaw in the previous proposals will be illustrated with Mirman's arguments,[6,7] supposedly supportive of the proposal by Aharonov and Susskind[5] for producing coherent superpositions of charge eigenstates. Mirman's argument can be set in the context of a Stern–Gerlach experiment involving two magnets and a beam of spin-1/2 particles. The coherence properties of the particle states are under investigation.

Denote the particle Hilbert space basis (eigenstates of an observable such as σ_z) by $|u\rangle_p$ and $|d\rangle_p$; similarly, each magnet Hilbert space has only two possibilities, e.g., $|\,u\rangle_1$ and $|\,d\rangle_1$ for the first magnet. Initially the global state is taken as (we suppress the state of the second magnet in what follows)

$$\psi(0) = |\,u\rangle_p(l_u\,|\,u\rangle_1 + l_d\,|\,d\rangle_1) \tag{29}$$

Upon interaction with the first magnet, the global state evolves to the form

$$\begin{aligned}\psi(t) &= l_u(m_u\,|\,u\rangle_p\,|\,u\rangle_1 + m_d\,|\,d\rangle_p\,|\,d\rangle_1)\\ &\quad + l_d(n_u\,|\,u\rangle_p\,|\,d\rangle_1 + n_d\,|\,d\rangle_p\,|\,u\rangle_1)\\ &= |\,u\rangle_p(l_u m_u\,|\,u\rangle_1 + l_d n_u\,|\,d\rangle_1)\\ &\quad + |\,d\rangle_p(l_d n_d\,|\,u\rangle_1 + l_u m_d\,|\,d\rangle_1)\end{aligned} \tag{30}$$

Suppose now that

$$l_u m_u = D l_d n_d \tag{31}$$

and

$$l_d n_u = D l_u m_d \tag{32}$$

Then (30) is factorizable,

$$\psi(t) = E(D\,|\,u\rangle_p + |\,d\rangle_p)(l_d n_d\,|\,u\rangle_1 + l_u m_d\,|\,d\rangle_1) \tag{33}$$

where E is a normalization factor given by

$$E = (|\,D\,|^2 + 1)^{-1/2}(|\,l_d n_d\,|^2 + |\,l_u m_d\,|^2)^{-1/2} \tag{34}$$

The reduced density operator $\rho_p(t)$ for the particle is given by

$$\begin{aligned}\rho_p(t) &= \mathrm{Tr}_1(P_{\psi(t)})\\ &= E^2\,\mathrm{Tr}_1(P_{(D|u\rangle_p+|d\rangle_p)} \otimes P_{(l_d n_d|u\rangle_1+l_u m_d|d\rangle_1)})\\ &= (|\,D\,|^2 + 1)^{-1}\,P_{(D|u\rangle_p+|d\rangle_p)}\end{aligned} \tag{35}$$

This pure state is a coherent superposition of $|\,u\rangle_p$ and $|\,d\rangle_p$. The assumption of factorizability of the final global state, expressed in (31) and (32), is an essential ingredient in Mirman's argument. Note now that if either $l_u = 0$ or $l_d = 0$ in (29), then (31)–(33) show that $\psi(t) = 0$. Thus the initial magnet state must be a coherent superposition ($l_u \neq 0$ and $l_d \neq 0$ both true) in order for Mirman's scheme to yield any nonzero final global state, in particular one leading to a coherent superposition like (35) for the particle state. Thus, if the initial particle state obeys the state restrictions, subsequent violation of state restrictions for the particle states necessarily entails a similar violation for the initial magnet state; Mirman seems to have been aware of this requirement. If the state restrictions are logically necessary for the superselection rule, Mirman's proposal begs the question. If they are not logically necessary, it does not challenge the superselection rule, since there was no concurrent violation of the observable restrictions; even if there had been, his proposal would still beg the question.

The existing proposals for superselection rule violation are schemes for the production of illegal quantum states. None of these schemes pays any attention to the fact that if the list of observables is restricted to those commuting with Q then it would be impossible to detect the illegal state, i.e., the observable restrictions alone are in fact sufficient for the superselection rule. Thus none of these proposals seriously challenges the superselection rules. Of course this criticism is couched in a context wherein state restrictions and observable restrictions are each sufficient but not necessary for the superselection rule. However, even if the viewpoint regarding these as necessary conditions is endorsed, there is no challenge, since the question is begged. The conclusion appears to be that regardless of the logical status of the state and observable restrictions, no consistent proposal for superselection rule violation has been made to date.

4. ALTERNATIVE DECOMPOSITIONS OF PERMISSIBLE DENSITY OPERATORS

Consider a mixed ensemble of quantum systems; the density operator ρ might be given in the form

$$\rho = \sum_k w_k \rho_k \tag{36}$$

where the real numbers $w_k \geqslant 0$ can be interpreted as relative weights on the ensemble; this interpretation goes all the way back to von Neumann.[9] Clearly, if each ρ_k commutes with Q, then so does ρ: thus a permissible ensemble can be formed by mixing permissible subensembles. What if some of the ρ_k in (36) do not commute with Q; is this possible with ρ commuting with Q? This mathematical problem will now be investigated.

In discussing the alternative mathematical decompositions of a given density operator ρ in the context of superselection rules it is helpful to note that there are altogether eight cases of interest depending on whether or not ρ is permissible, if the contemplated decomposition is a spectral expansion, or whether the projections making up the decomposition are permissible or not. The discussion will be broken into two areas: spectral and nonspectral decompositions.

All density operators are Hermitian; moreover, all density operators have a discrete spectrum. The latter assertion follows since any density operator is totally continuous (trace class).[10] The spectral theorem for compact Hermitian operators[11] applied to any density operator ρ with nondegenerate spectrum then asserts the unique existence of a family of operators P_k such that

$$\rho = \sum_k a_k P_k \tag{37}$$

The P_k are orthogonal projection operators onto the eigenspaces of ρ; each a_k is a distinct ρ eigenvalue. Any decomposition of the form (37) will be called *spectral*. The spectral theorem then asserts that (37) is the only decomposition of ρ into orthogonal projections with ρ eigenvalue coefficients.

In the sequel we shall let the charge operator Q be the only superselection operator under consideration. The spectrum of the charge operator is evidently infinitely degenerate; thus, in a representation in which Q is diagonal, the matrix representatives of particular operators will be infinite-dimensional. When these matrices are explicitly written out, a convention of displaying only the largest submatrix with nonzero entry rows and columns will be employed. With this convention, the matrices will appear to be finite-dimensional, whereas in actual fact they are not.

The first type of spectral decomposition to be considered is that of a nonpermissible density operator. This can be a linear combination of either permissible or nonpermissible projections. Since a linear combination of block-diagonal matrices is again block-diagonal, not every projection can be permissible if ρ is nonpermissible. For example, consider the following density operator:

$$\rho = \tfrac{1}{4}P_{\phi_1} + \tfrac{1}{4}P_{\phi_2} + \tfrac{1}{2}P_{\phi_3} \tag{38}$$

where

$$\begin{aligned} \phi_1 &= (1/\sqrt{2})(\,|\,q_1 1\rangle + |\,q_2 1\rangle) \\ \phi_2 &= (1/\sqrt{2})(\,|\,q_1 2\rangle + |\,q_2 2\rangle) \\ \phi_3 &= |\,q_3 1\rangle \end{aligned} \tag{39}$$

Here, q_1, q_2, and q_3 are distinct eigenvalues of Q. Using the orthonormality of the $|\,qd_q\rangle$, i.e., $\langle qd_q \,|\, q'd'_{q'}\rangle = \delta_{qq'}\delta_{d_q d'_q}$, it is easy to check that this is a spectral expansion of ρ. The ρ given here is degenerate: ϕ_1 and ϕ_2 both belong to ρ eigenvalue 1/4; ϕ_3 belongs to ρ eigenvalue 1/2. This degeneracy is of no consequence for what we wish to establish. Note that ρ is indeed a possible valid density operator since it has a positive spectrum (hence ρ is positive), it is Hermitian, and it has unit trace. Two of the projections in (38) are nonpermissible, however, since each of the vectors ϕ_1, ϕ_2 in (39) violates the state restrictions. Thus we have an example of a spectral expansion of a nonpermissible ρ involving a combination of permissible and nonpermissible projections.

Since the labeling of matrices in problems of this sort can lead to some confusion, we shall digress for a moment to display the operator in (38) in matrix form in Q representation, employing our convention. The column labels have been indicated in a horizontal row above the matrix; similarly, the labels of those rows containing at least one nonzero element have been written out down the left margin of the matrix. Ellipsis marks have been inserted to indicate the position of the columns (rows) with all entries equal to zero:

$$\begin{array}{c} \\ q_1 1 \\ q_1 2 \\ \vdots \\ q_2 1 \\ q_2 2 \\ \vdots \\ q_3 1 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccc} q_1 1 & q_1 2 & \cdots & q_2 1 & q_2 2 & \cdots & q_3 1 & \cdots \end{array} \\ \left[\begin{array}{ccccc} \frac{1}{8} & 0 & \frac{1}{8} & 0 & 0 \\ 0 & \frac{1}{8} & 0 & \frac{1}{8} & 0 \\ \frac{1}{8} & 0 & \frac{1}{8} & 0 & 0 \\ 0 & \frac{1}{8} & 0 & \frac{1}{8} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} \end{array}\right] \end{array} = \rho \qquad (40$$

The second type of spectral decomposition is that of a permissible density operator. As in the nonpermissible case, the logical possibilities include linear combinations of either permissible or nonpermissible projections. An example of a spectral decomposition of a permissible ρ involving no nonpermissible projections is easy to find. Consider the operator

$$\rho = \frac{\sqrt{2}+1}{4\sqrt{2}} P_{\phi_1} + \frac{\sqrt{2}-1}{4\sqrt{2}} P_{\phi_2} + \frac{1}{2} P_{\phi_3} \qquad (41)$$

where

$$\begin{aligned} \phi_1 &= \tfrac{1}{2}(2+\sqrt{2})^{1/2} \mid q_1 1\rangle + \tfrac{1}{2}(2-\sqrt{2})^{1/2} \mid q_1 2\rangle \\ \phi_2 &= \tfrac{1}{2}(2-\sqrt{2})^{1/2} \mid q_1 1\rangle - \tfrac{1}{2}(2+\sqrt{2})^{1/2} \mid q_1 2\rangle \\ \phi_3 &= \mid q_2 1\rangle \end{aligned} \qquad (42)$$

It is easy to verify that the ρ given by (41) is a positive Hermitian operator of unit trace and that (41) and (42) indeed constitute a spectral expansion. Each projection in (41) is permissible since from (42), $\phi_1 \in H_{q_1}$, $\phi_2 \in H_{q_1}$, and $\phi_3 \in H_{q_2}$, where H_q denotes the q eigenspace of Q. Note that this ρ is nondegenerate; thus (41) is the only spectral expansion for this ρ.

It is natural to wonder, under the assumption that ρ has a nondegenerate spectrum, if the *spectral* expansion of a permissible density operator is always in terms of permissible projections. This is easily shown to be the case: the demonstration begins with the observation that the permissibility of ρ entails that ρ and Q share a complete set of eigenvectors, $\{| rqd_{rq}\rangle\}$, so that

$$\rho = \sum_{rqd_{rq}} w_r \mid rqd_{rq}\rangle\langle rqd_{rq} \mid \tag{43}$$

and

$$Q = \sum_{rqd_{rq}} q \mid rqd_{rq}\rangle\langle rqd_{rq} \mid \tag{44}$$

Each of these is a spectral expansion. Equation (43) can be written in a more familiar form as follows:

$$\rho = \sum_r w_r \sum_{qd_{rq}} \mid rqd_{rq}\rangle\langle rqd_{rq} \mid \equiv \sum_r w_r P_r \tag{45}$$

Now if ρ has a nondegenerate spectrum, then for each w_r there is only one eigenvector $\mid rqd_{rq}\rangle$ satisfying

$$\rho \mid rqd_{rq}\rangle = w_r \mid rqd_{rq}\rangle \tag{46}$$

Thus the degree of degenracy of each w_r is unity, so that in (46) we may set $q = q_r$ and $d_{rq} = 1$. The projections P_r onto the ρ eigenspaces thus take the simple form, for all r,

$$P_r = \mid rq_r1\rangle\langle rq_r1 \mid \tag{47}$$

From this and the fact that each $\mid rqd_{rq}\rangle$ is a simultaneous eigenvector of Q it follows that each P_r commutes with Q. Therefore the spectral expansion of a permissible density operator possessing a nondegenerate spectrum is always in terms of permissible projections, as we wished to show.

One of the key points in the above demonstration is the uniqueness of the spectral decomposition of a Hermitian operator in the absence of degeneracies. In this regard note that

$$P_r \equiv \sum_{qd_{rq}} \mid rqd_{rq}\rangle\langle rqd_{rq} \mid \tag{48}$$

commutes with Q. Thus it appears that each P_r can be permissible even in the presence of degeneracies; in the nondegenerate case the spectral expansion is unique and thus P_r is rigorously permissible. However, with degeneracies and a consequent nonuniqueness of the spectral decomposition, we should not expect this to be true necessarily. Indeed it is not difficult to find counter-examples.

For example, consider the following permissible density operator:

$$\rho = \tfrac{1}{4} \mid q_1 1\rangle\langle q_1 1 \mid + \tfrac{1}{2} \mid q_1 2\rangle\langle q_1 2 \mid + \tfrac{1}{4} \mid q_2 1\rangle\langle q_2 1 \mid \tag{49}$$

This is obviously a spectral decomposition: the coefficients are eigenvalues of ρ and the projections are orthogonal. As defined, ρ is diagonal in the Q representation, so the eigenvalues are 1/4 and 1/2. Already the spectrum of ρ is manifestly degenerate. Now an alternative decomposition of ρ is

$$\rho = \tfrac{1}{4}P_{\phi_1} + \tfrac{1}{4}P_{\phi_2} + \tfrac{1}{2}P_{\phi_3} \tag{50}$$

where

$$\begin{aligned} \phi_1 &= (1/\sqrt{2}) \mid q_1 1\rangle + (1/\sqrt{2}) \mid q_2 1\rangle \\ \phi_2 &= -(1/\sqrt{2}) \mid q_1 1\rangle + (1/\sqrt{2}) \mid q_2 1\rangle \\ \phi_3 &= \mid q_1 2\rangle \end{aligned} \tag{51}$$

This, too, is a spectral decomposition: the coefficients are all eigenvalues of ρ, all ϕ_i are eigenvectors of ρ, and all the P_{ϕ_i} satisfy $P_{\phi_i}P_{\phi_k} = \delta_{ik}P_{\phi_i}$. The ρ eigenvalue 1/4 is twofold degenerate. Equation (50) constitutes our counterexample; P_{ϕ_1} and P_{ϕ_2} do not commute with Q, whereas ρ is permissible. Thus, if a permissible density operator ρ has a degenerate spectrum, it is a priori conceivable to subdivide an ensemble characterized by ρ into non-permissible subensembles, based solely on a consideration of alternative *spectral* decompositions of ρ.

The cases involving nonspectral decompositions will now be investigated. Even in the absence of degeneracies, it is obvious that the *nonspectral* expansion of a density operator is not unique. The case of nonspectral decompositions is therefore potentially more interesting in the context of superselection rules. We have already determined that the spectral decomposition of a nondegenerate-spectrum permissible density operator can not possibly introduce any difficulties in a superselection rule context: the constituent orthogonal projections are always permissible. This will not be the case for the nonspectral decompositions of permissible density operators with nondegenerate spectra, as will now be shown.

We shall not dwell long upon the rather uninteresting case of a nonspectral decomposition of a nonpermissible ρ. Obviously, it cannot be in terms of permissible projections alone, since any linear combination of them would be permissible, a contradiction. The only other possibility is that it is in general in terms of nonpermissible projections. The situation is analogous to the case of the spectral decomposition of nonpermissible density operators.

The more interesting situation involves the nonspectral decompositions of a permissible ρ. There are two possibilities that are characterized by the "permissibility status" of the projections making up the decomposition. The first case is a nonspectral decomposition of a permissible ρ into a linear combination of permissible projections; we shall not address ourselves to this case either, since it is of no particular interest in the context of superselection rules. The other possibility, a nonspectral decomposition of a permissible ρ consisting of a linear combination of nonpermissible projections is of considerable interest in this context. It will be established that such a decomposition is possible.

We begin with a mathematical characterization of the general decomposition (i.e., spectral or nonspectral) of a permissible density operator ρ

$$\rho = \sum_{ql_q} r_{ql_q} P_{\psi_{ql_q}} \tag{52}$$

where

$$| \psi_{ql_q} \rangle = \sum_{d_q} a_{ql_q d_q} \, | qd_q \rangle \tag{53}$$

is a unit vector, i.e., $\| \psi_{ql_q} \| = 1$. Here ψ_{ql_q} is the l_qth vector in the Q eigenspace H_q use to form ρ via (52). It is not necessarily equal to $| qd_q \rangle$; if, however, for every l_q there exists a d_q such that $\psi_{ql_q} = | qd_q \rangle$, then (52) becomes a spectral decomposition. We have already investigated that situation.

A straightforward calculation using (52) and (53) gives

$$\rho = \sum_{ql_q} r_{ql} \sum_{q' d_q d'_{q'}} a_{ql_q d_q} a^*_{q' l_{q'} d'_{q'}} \delta_{qq'} \, | qd_q \rangle \langle q' d'_{q'} | \tag{54}$$

The problem now is to find an alternative decomposition of (52), of the form

$$\rho = \sum_i V_i P_{\phi_i} \tag{55}$$

where the ϕ_i, unlike the ψ_{ql_q} of (53), do not in general obey the state restrictions, i.e., where

$$\phi_i = \sum_{qd_q} C_{iqd_q} \, | qd_q \rangle \tag{56}$$

This will be done employing a technique introduced by Schrödinger.[12] Combining (55) and (56) in a manner analogous to that which led to (54), there results an expression for ρ similar to (54), but involving the V_i and C_{iqd_q}. Equating this with (54) gives

$$\sum_i V_i C_{iqd_q} C^*_{iq'd'_{q'}} = \delta_{qq'} \sum_{l_q} r_{ql_q} a_{ql_q d_q} a^*_{q' l_{q'} d'_{q'}} \tag{57}$$

Define

$$g_{iqd_q} \equiv \frac{(V_i)^{1/2}}{\sum_{l_q} a_{ql_q d_q} (r_{ql_q})^{1/2}} C_{iqd_q} \tag{58}$$

The g_{iqd_q} are well defined provided (58) involves no divisions by zero. They are not totally arbitrary since (57) links them essentially with a condition on the C_{iqd_q}; the condition the g_{iqd_q} must satisfy in order that (58) may be used to determine the unknown C_{iqd_q} is of fundamental importance. If all the V_i are real, it is given by the following expression:

$$\sum_i g_{iqd_q} g^*_{iq'd'_{q'}} = \left(\sum_{l_q} r_{ql_q} a_{ql_q d_q} a^*_{q' l_{q'} d'_{q'}} \right) \times \left[\sum_{l_q l'_{q'}} a_{ql_q d_q} a^*_{q' l'_{q'} d'_{q'}} (r_{ql_q} r_{q' l'_{q'}})^{1/2} \right]^{-1} \delta_{qq'} \tag{59}$$

The C_{iqd_q} will be determined by (58) if a set of g_{iqd_q} satisfying (59) can be found and if the V_i can be determined. The V_i are found using the normalization of ϕ_i. This, together with (56), places a subsidiary condition on the C_{iqd_q},

$$\sum_{qd_q} C^*_{iqd_q} C_{iqd_q} = 1 \tag{60}$$

Substitution of (58) into this gives the desired result

$$V_i = \sum_{qd_q} | g_{iqd_q} |^2 \sum_{l_q l'_q} a_{ql_q d_q} a^*_{ql'_q d_q} (r_{ql_q} r_{ql'_q})^{1/2} \tag{61}$$

The problem is therefore solved; it has been shown that the alternative decomposition (55) is determinable provided a set of quantities g_{iqd_q} satisfying (59) can be found. It is convenient to think of this set as the set of components of a set of vectors $\mathbf{g}_{qd_q}$. Equation (59) then asserts that these vectors are in general orthogonal only for different q. The dimensionality of the $\mathbf{g}_{qd_q}$ is equal to the number of different ϕ_i in the sought expansion (55).

Therefore there is a prescription for the discovery of alternative nonspectral decompositions of a permissible density operator in terms of nonpermissible projections. The general conditions that guarantee the existence of a set of $\mathbf{g}_{qd_q}$ permitting the rendition of this decomposition will not be studied; for present purposes, the above algorithm and an example of its successful use will suffice. Thus our attentions now turn to the investigation of a specific permissible density operator. Consider

$$\rho = r_{q_1 1} P_{\psi_{q_1 1}} + r_{q_1 2} P_{\psi_{q_1 2}} + r_{q_2 1} P_{\psi_{q_2 1}} \tag{62}$$

where

$$\psi_{q_1 1} = (1/\sqrt{2})(|\, q_1 1\rangle + |\, q_1 2\rangle), \qquad \psi_{q_1 2} = |\, q_1 1\rangle, \qquad \psi_{q_2 1} = |\, q_2 1\rangle \tag{63}$$

and $r_{q_1 1} = r_{q_1 2} = 1/4$, $r_{q_2 1} = 1/2$. Thus the $a_{q l_q d_q}$ of (53) are

$$\begin{aligned} a_{q_1 11} &= 1/\sqrt{2}, \qquad & a_{q_1 12} &= 1/\sqrt{2}, \qquad & a_{q_1 13} &= 0,\ldots \\ a_{q_1 21} &= 1, & a_{q_1 22} &= 0, & a_{q_1 23} &= 0,\ldots \\ a_{q_2 11} &= 1, & a_{q_2 12} &= 0, & a_{q_2 13} &= 0,\ldots \end{aligned} \tag{64}$$

As defined, the vectors in (63) all obey the state restrictions: $\psi_{q_1 1} \in H_{q_1}$, $\psi_{q_1 2} \in H_{q_1}$, and $\psi_{q_2 1} \in H_{q_2}$. The matrix of the operator in (62) is therefore block-diagonal in Q representation. It will be seen later that it also constitutes a legitimate density operator and that (62) is not a spectral expansion. A different nonspectral expansion of ρ in terms of nonpermissible projections is now desired.

The first step in finding this is the determination of the $\mathbf{g}_{q d_q}$. There will be three such vectors: $\mathbf{g}_{q_1 1}$, $\mathbf{g}_{q_1 2}$, and $\mathbf{g}_{q_2 1}$. An alternative decomposition of the form

$$\rho = V_1 P_{\phi_1} + V_2 P_{\phi_2} + V_3 P_{\phi_3} \tag{65}$$

is sought so that the $\mathbf{g}_{q d_q}$ vectors are three-dimensional. It is convenient to let (59) be the definition of an inner product for these vectors; denote this by $\mathbf{g}_{q d_q} \cdot \mathbf{g}_{q' d'_{q'}}$. From (59) it is an easy matter to determine the conditions the $\mathbf{g}_{q d_q}$ must satisfy:

$$\begin{aligned} \mathbf{g}_{q_1 1} \cdot \mathbf{g}_{q_1 1} &= 3/(1+\sqrt{2})^2, \qquad & \mathbf{g}_{q_1 1} \cdot \mathbf{g}_{q_1 2} &= 1/(1+\sqrt{2}) \\ \mathbf{g}_{q_1 2} \cdot \mathbf{g}_{q_1 2} &= 1, & \mathbf{g}_{q_1 1} \cdot \mathbf{g}_{q_2 1} &= 0 \\ \mathbf{g}_{q_2 1} \cdot \mathbf{g}_{q_3 1} &= 1, & \mathbf{g}_{q_1 2} \cdot \mathbf{g}_{q_2 1} &= 0 \end{aligned} \tag{66}$$

Thus, $\mathbf{g}_{q_2 1}$ is orthogonal to the plane formed by $\mathbf{g}_{q_1 1}$ and $\mathbf{g}_{q_1 2}$. Moreover, $\mathbf{g}_{q_1 1}$ and $\mathbf{g}_{q_1 2}$ are not orthogonal. Finally, all the vectors, save $\mathbf{g}_{q_1 1}$, are unit vectors. The following vectors meet all the stipulations of (66):

$$\mathbf{g}_{q_1 1} = \frac{1}{\sqrt{2}(1+\sqrt{2})}\begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}, \qquad \mathbf{g}_{q_1 2} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \qquad \mathbf{g}_{q_2 1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \tag{67}$$

Then the r_{qd_q}, $a_{ql_qd_q}$, and g_{iqd_q} being known, the form (65) is determined using (56), (58), and (61). The result is

$$\begin{aligned} V_1 &= V_2 = \tfrac{3}{8}, \qquad V_3 = \tfrac{1}{4} \\ \phi_1 &= -(1/\sqrt{6}) \mid q_1 1\rangle - (1/\sqrt{6}) \mid q_1 2\rangle + \sqrt{\tfrac{2}{3}} \mid q_2 1\rangle \\ \phi_2 &= (1/\sqrt{6}) \mid q_1 1\rangle + (1/\sqrt{6}) \mid q_1 2\rangle + \sqrt{\tfrac{2}{3}} \mid q_2 1\rangle \\ \phi_3 &= \mid q_1 1\rangle \end{aligned} \tag{68}$$

Note that ϕ_1 and ϕ_2 do not obey the state restrictions. The expansion is also nonspectral since $\langle \phi_1, \phi_3 \rangle = -\langle \phi_2, \phi_3 \rangle \neq 0$. It is easily verified that the new decomposition is correct by calculating the projections P_{ϕ_i} with (68) and substituting into (65). This result can be compared with an analogous calculation using (62) and (63). The results of both these calculations for this example are

$$\begin{aligned} \rho = &\tfrac{3}{8} \mid q_1 1\rangle\langle q_1 1 \mid + \tfrac{1}{8} \mid q_1 1\rangle\langle q_1 2 \mid + \tfrac{1}{8} \mid q_1 2\rangle\langle q_1 1 \mid \\ &+ \tfrac{1}{8} \mid q_1 2\rangle\langle q_1 2 \mid + \tfrac{1}{2} \mid q_2 1\rangle\langle q_2 1 \mid \end{aligned} \tag{69}$$

In matrix form (with the convention regarding infinite matrices),

$$\rho = \begin{pmatrix} \frac{3}{8} & \frac{1}{8} & 0 \\ \frac{1}{8} & \frac{1}{8} & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix} \tag{70}$$

This operator is familiar from an earlier example, in the discussion of spectral expansions of permissible density operators [cf. (41) and (42)]. In other words, (41) is the spectral expansion of the permissible density operator just investigated. Thus, three different decompositions of the same permissible density operator have been found, one spectral and two nonspectral, one of the latter of which was in terms of nonpermissible projections.

Therefore, the general decomposition (36) of a permissible density operator can involve nonpermissible constituents ρ_k. Moreover, it is mathematically conceivable, and consistent with the standard interpretation of such a decomposition, to regard a permissible ensemble as consisting of nonpermissible subensembles. If the decomposition is spectral, ρ must have degenerate spectrum for any ρ_k to be nonpermissible; the nonspectral decompositions do not require this. It would appear that state restriction violation is a possibility if some consistent scheme for selection of the nonpermissible subensembles exists.

5. SUMMARY AND CONCLUSIONS

Previous proposals for superselection rule violation consist of schemes for the preparation of illegal (nonpermissible, nonphysical) quantum states. The tacit assumption is that the state restrictions are a necessary condition for the superselection rule. It is argued here that both the state and the observable restrictions are each sufficient but not necessary conditions for the superselection rule, contrary to the usual interpretation. Thus the previous proposals are properly understood as state restriction violation proposals. It has been known for some time that each of these proposals begs the question by necessarily requiring illegal states initially.

A new proposal for state restriction violation has emerged. The stimulus for this was the problem of ensemble subdivision of an ensemble of quantum systems with permissible quantum state. By considering alternative mathematical decompositions of permissible density operators, it was shown that it is a priori conceivable to subdivide a permissible ensemble into nonpermissible subensembles, a heretofore unrecognized possibility. It is recognized that the present proposal is devoid of a specific prescription for bringing about the required subdivision. The intent here is to show the mathematical consistency of so doing. If the subdivision is impossible, the argument for that will have to consider the effect of superselection rules on the dynamics of the subdivision process.

Further argument on the logical status of the state and observable restrictions is postponed to Part II of this work, as is a specific dynamical argument regarding the ensemble subdivision problem.

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