Superselection Rules; Old and New (*).

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Summary. — This paper is a historical review of the development of the notion of superselection rule starting from the recognition in 1952 of the charge and univalence superselection rules. Some applications to environmentally induced superselection rules in the last decade are briefly described.

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1. – Introduction.

Mesoscopic physics offers us the delicious prospect of experimental situations half-way between the microscopic and the macroscopic in which quantum-mechanical interference effects are important, but also other situations in which decoherence processes destroy the relative phases of states so as to produce classical behavior. We may expect to find in mesoscopic physics a rich family of tests of the basic ideas of quantum mechanics and of its interpretation. In particular, the question of what is observable and what is unobservable will be salient; it is here that the notion of superselection rule emerges.

In this paper, I will review some of the history of the notion of a superselection rule. Some of the material is so old that it may have been forgotten. That is one excuse for presenting it—a more significant reason is that this old stuff provides the background for exciting recent developments and a framework for the discussion of future experiments.

2. – von Neumann's book and Wigner's remark.

von Neumann's book, *Mathematische Grundlagen der Quantenmechanik* published in 1932 made many contributions to its subject:

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a) It gave an *ab initio* treatment of abstract Hilbert space, and the linear operators acting on it. This put non-relativistic quantum mechanics on a sound mathematical footing.

b) It gave a precise mathematical interpretation to the notion of quantum-mechanical observable: To each observable there corresponds a self-adjoint operator in the Hilbert space of states.

c) It gave a careful discussion of the statistical interpretation of quantum-mechanics and undertook to prove, under certain assumptions, the impossibility of a hidden-variables interpretation of quantum mechanics (von Neumann's Impossibility Theorem).

d) It analyzed the process of measurement in quantum mechanics under the assumption that the measuring apparatus is also governed by the laws of quantum mechanics.

What is of primary interest for the purposes of this article is the set of assumptions made by von Neumann for the proof of the Impossibility Theorem. Almost casually he says, «... it is appropriate to assume» that every self-adjoint operator is the operator of some observable [1]. To emphasize: not only does he assume that every observable determines a self-adjoint operator, but also that every self-adjoint operator is the self-adjoint operator of some observable. So far as I know, this latter assumption was not questioned publicly in the two decades that followed the publication of von Neumann's book. However, at the end of the 1940's when I was studying Wigner's analysis of symmetry in quantum mechanics under the tutelage of Bargmann and Wigner, Wigner was already considering the possibility that operators such as Q, the total electric charge, might commute with all observables, thus invalidating von Neumann's assumption. It was characteristic of the situation envisaged by Wigner that the Hilbert space of states, $\mathscr{H}$, would be a direct sum of subspaces, $\mathscr{H}_j$:

$$\mathscr{H} = \bigoplus_j \mathscr{H}_j$$

(later called coherent subspaces or superselection sectors) in which the superposition principle is valid but that a linear combination, $\alpha\psi_1 + \beta\psi_2$, of states ψ_1 and ψ_2 from two distinct coherent subspaces would not be physically realizable except as a mixture with the density matrix

$$|\alpha|^2\psi_1 \otimes \bar{\psi}_1 + |\beta|^2\psi_2 \otimes \bar{\psi}_2 .$$

An alternative equivalent description is that the relative phase of β and α in $\alpha\psi_1 + \beta\psi_2$ is not observable.

WBW checked that the Wignerian analysis of symmetry generalizes to such a situation. Recall that Wigner's analysis of quantum-mechanical theories invariant under the Poincaré (= inhomogeneous Lorentz) group $\mathscr{P}_+^\uparrow$ led to representations up to a factor $\{a, \Lambda\} \to U(a, \Lambda)$ satisfying the multiplication law

$$U(a_1, \Lambda_1)\, U(a_2, \Lambda_2) = \omega(a_1, \Lambda_1;\, a_2, \Lambda_2)\, U(a_1 + \Lambda_1 a_2, \Lambda_1\Lambda_2),$$

where $|\omega(a_1, \Lambda_1, a_2, \Lambda_2)| = 1$. In the more general situation envisaged by Wigner, ω can differ in different coherent subspaces, so the reduction from representations up to a factor to true representations of the covering group has to be carried out on each coherent subspace separately.

The first public occasion on which von Neumann's assumption was discussed was a conference organized by Enrico Fermi in Chicago in September 1951. There was at that time a considerable interest in the possible transformation laws of spinors under inversions and in the question whether such transformation laws could give meaning to a notion of intrinsic parity of spin-(1/2) elementary particles. A year earlier Yang and Tiomno [2] and Zharkov [3] had proposed that one should distinguish four different transformation laws for a Dirac spinor under space-inversion i_s:

$$(i_s\psi)(t,\boldsymbol{x}) = \pm\gamma^0\psi(t,-\boldsymbol{x}), \qquad i_s^2 = +1, \tag{2.1}$$

$$(i_s\psi)(t,\boldsymbol{x}) = \pm i\gamma^0\psi(t,-\boldsymbol{x}), \qquad i_s^2 = -1. \tag{2.2}$$

The idea was that if the spinor fields for p, n, $\mu^\pm$, $e^\pm$, $\nu,\bar\nu$ are assigned one of these transformation laws under space-inversion and then combined to form interaction terms either among themselves or with other fields, some interaction terms would be excluded by parity conservation.

Fermi scheduled a special session at the conference devoted to these ideas and began it by emphasizing that the distinctions among the four kinds of spinors can be regarded as analogues of the distinction between scalars and pseudo-scalars and between vectors and pseudo-vectors. He also posed the question how the different classes of spinors might be distinguished experimentally. The proceedings of the conference give some further details of Fermi's talk as well as brief summaries of what Yang and Wigner said. However, I am left with the impression that not everyone understood what Wigner had to say about von Neumann's assumption. That is fortified by the last paragraph of the session summary [4]:

«Requiem was read by E. Teller who cited the a propos anecdote of a candidate for a doctor's in philosophy who made a statement he presumed to be true. Upon being asked by a professor on the examining board, "In which universe?" he responded, "Which which?"».

Fortunately, there was at least one person in the audience who got the message: Gian Carlo Wick. I have been told that he said to Eugene: «Eugene, these arguments have to be published and I volunteer to write the first draft». So was born, W^3 [5]. Before I embark on a description of what W^3 contained and what it did not contain, another historical remark is in order.

For mathematical reasons, Cartan had already introduced the distinction between (2.1) and (2.2) in 1938 in his lectures on spinors [6]. Cartan proposed to extend the notion of covering group from $SO(3)$ to $O(3)$. For $SO(3)$, the universal covering group is $SU(2)$, where $A \in SU(2)$ corresponds to $R(A) \in SO(3)$, with

$$R(A) = R(-A).$$

When the operation of space-inversion represented by the 3×3 matrix, -1, is adjoined to $SO(3)$ to give $O(3)$, one can construct a covering group that agrees with $SU(2)$ over $SO(3)$ in two ways: if i_s is an element of the covering group such that $R(i_s) = -1$, then there are two non-isomorphic possibilities: $i_s^2 = \pm 1$; this is the distinction between (2.1) and (2.2) expressed in terms of covering groups. Cartan called the quantities transforming in these distinct manners spinors of the first and second kinds.

Wigner had shocked the Chicago conference by discussing the possibility that certain relative phases of quantum-mechanical states are unobservable. W^3 systematized the discussion of this possibility by introducing the notion of a *superselection rule*, an exact conservation law for a self-adjoint operator, A, with the property that the relative phase of eigenfunctions belonging to any pair of distinct eigenvalues of A is unobservable. What they actually said was:

«We shall say that a superselection rule operates between subspaces if there are neither spontaneous transitions between their state vectors (*i.e.* if a selection rule operates between them) and if, in addition to this, there are no measurable quantities with finite matrix elements between their state sectors.»

W^3 contained several more things:

a) arguments that there is a univalence superselection rule and an electric-charge superselection rule.

b) A suggestion that baryon number might also define a superselection rule.

c) A discussion of the notions of parity and relative parity for particles under the assumption that only the univalence superselection rule operates or that both univalence and charge superselection rules operate.

I use the term univalence superselection rule to mean that there is an operator commuting with all observables that is $+1$ on the subspace of states where the representation of the rotation group is single-valued (integer angular momentum) and -1 on the subspace where it is double-valued (half-odd integer angular momentum). I was not very successful in convincing W^2 that this is good terminology but I persist. (They preferred «fermion-boson superselection rule».)

W^3 offered a proof of the univalence superselection rule under the assumption that the system is invariant under time inversion $i_t:\{t, \boldsymbol{x}\} \to \{-t, \boldsymbol{x}\}$ and that the anti-unitary operator of time inversion $U(i_t)$ satisfies

$$U(i_t)^2 = (-1)^{2j}.$$

The argument could not be simpler.

The iteration of time inversion on a state Ψ should yield a physically equivalent state $U(i_t)^2\Psi$, but if $(-1)^{2j}\Psi_A = \Psi_A$ and $(-1)^{2j}\Psi_B = -\Psi_B$, then $\Psi_A = \Psi_A + \Psi_B$ has to be physically equivalent to $\Psi_A - \Psi_B$ and $\Psi_A + i\Psi_B$ to $\Psi_A - i\Psi_B$. Then if C is any observable

$$(\Psi_A + \Psi_B, C(\Psi_A + \Psi_B)) = (\Psi_A - \Psi_B, C(\Psi_A - \Psi_B)),$$

so $(\Psi_A, C\Psi_B) + (\Psi_B, C\Psi_A) = 0$ or $\mathrm{Re}(\Psi_A, C\Psi_B) = 0$. Similarly,

$$(\Psi_A + i\Psi_B, C(\Psi_A + i\Psi_B)) = (\Psi_A - i\Psi_B, C(\Psi_A - i\Psi_B)),$$

so $i[(\Psi_A, C\Psi_B) - (\Psi_B, C\Psi_A)] = 0$ so $\mathrm{Im}(\Psi_A, C\Psi_B) = 0$.

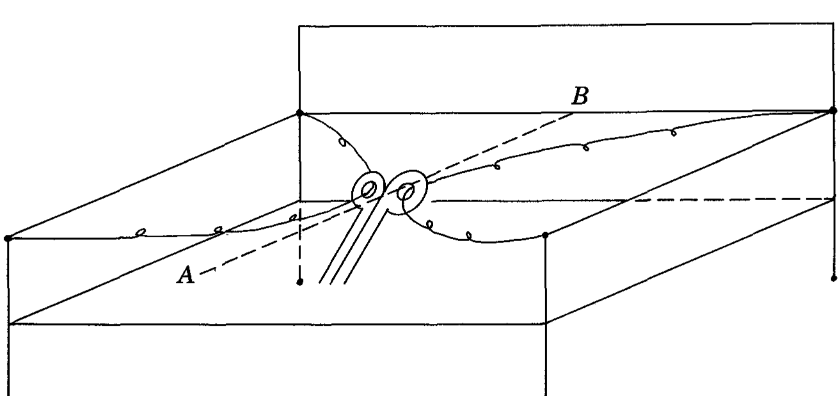
Thus, all off-diagonal matrix elements of the observable C vanish and $(-1)^{2j}$ defines a superselection rule. W^3 would have preferred to base the proof on invariance under $SO(3)$ alone, without making an assumption of time inversion invariance, but that would have required an extended discussion of the arbitrary phases occurring in the representation of $SO(3)$. Later on such an alternative proof was published in [7].

There were those who questioned the univalence superselection rule [8]. They pointed out that, if you split a system into two parts and rotate one of the parts through an angle of 2π, the resulting state of the composite system may have quite different properties from the original state of the composite system. A version of this idea was given an experimental test with two sub-beams of a beam of slow neutrons. The rotation of the spin of the neutron through an angle 2π was obtained by passing one of the two sub-beams through an appropriate magnetic field. The interference of the two final sub-beams was spectacularly different with and without the magnetic fields. These beautiful slow-neutron experiments are reviewed in [9] where further references may be found. As far as the relevance of these experiments to the univalence superselection rule is concerned, the standard response is that the experiments are beautiful, but they are not the ones involved in the univalence superselection rule where you must rotate the entire isolated system.

For the charge superselection rule a somewhat more involved argument is needed, but the conclusion is that the apparatus proposed to produce superposition states of different charges requires for its construction superposition states of different charges [10].

Next I would like to call attention to some geometrical constructions which exhibit a behavior like that seen for spinors under rotations through an angle $2\pi n$. Therefore, to some extent, these constructions make spinors less mysterious. So far as I know, it all began with a pedagogical demonstration used by Dirac in his lectures on quantum mechanics to illustrate the fact that the group $SO(3)$ is not simply connected. I first learned of it from a paper of Newman published in London in 1942 [11]. According to Newman, Dirac took two pieces of string which he attached to the arms of a chair, threading them through to handles of a pair of scissors as shown in fig. 1.

(This is my interpretation; for quite a different one see fig. B2.1, p. 228 in ref. [12].) He rotated the scissors about a horizontal axis, AB, by an angle 4π, and found that holding the scissors and the attachments to the chair fixed, he could disentangle the strings and restore them to their original configuration without cutting them. When the rotation was taken through an angle 2π instead of 4π, the disentanglement was impossible.



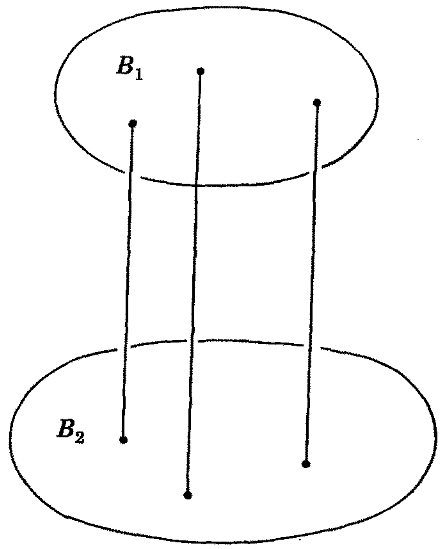


Fig. 2.

Newman also considered another configuration without scissors and proved a theorem about it. Given two convex bodies B_1 and B_2 connected by vertical parallel lines as shown in fig. 2. Rotate B_2 about a vertical axis by an angle $2\pi k$ where k is a positive integer, holding B_1 fixed and treating the lines as flexible strings attached to fixed points on B_1 and B_2. The strings are not allowed to pass through one another.

Theorem (Newman). If the number of strings $n \geqslant 3$ and k is even, the strings can be disentangled. If $n \geqslant 3$ and k is odd, they cannot.

When, in 1973, Misner, Thorne and Wheeler wrote the chapter on spinors for their grand treatise on gravitation they too abandoned chairs and scissors, but retained the strings which connect the object with its surroundings. In particular, they have a cube, some of whose corners are attached to the corners of the room in which it sits. I have followed [12] and attached a string to every corner. Newman's theorem holds in all these cases, and Misner, Thorne and Wheeler display how the disentanglement can be carried out for $n = 8$ [13]. (See fig. 3.)

Thus, for $n \geqslant 3$, these geometrical contraptions have one of the crucial features of a spinor: rotation through 2π does not give an equivalent configuration, but rotation through 4π does. The attachment provided by the strings somehow plays an analogous role to the coherent-phase relationships between the sub-beams in the neutron experiment described above.

W^3 did not offer a proof of the charge selection rule and their claim for experimental support was modest. They noted that:

«... multiplication of the state vector F by the operator $\exp[i\alpha Q]$ produces no physically observable modification of the state of a system of (mutually interacting) charged fields.

We can give no conclusive evidence for this assertion, and such evidence may in

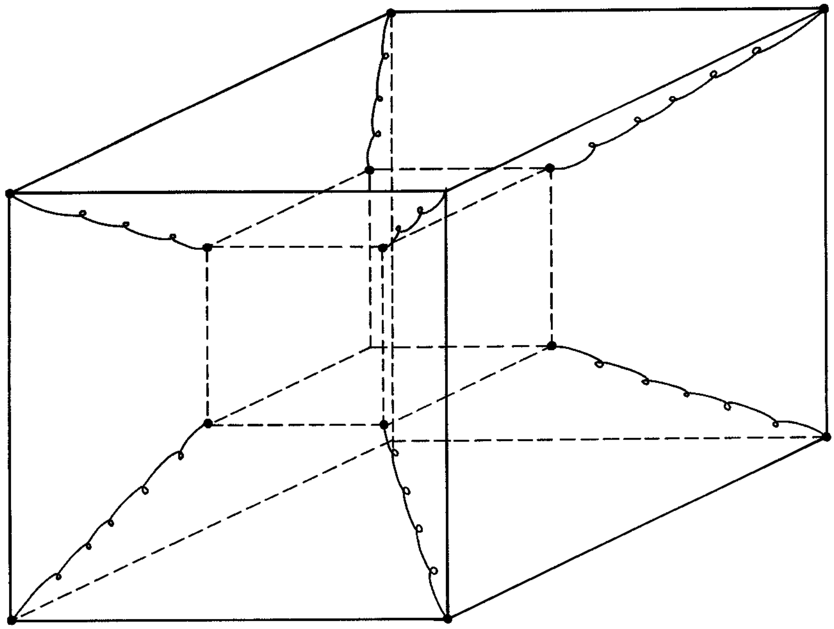


Fig. 3.

fact depend on a deeper understanding of the meaning of electric charges which we still lack. Assuming that the assertion is correct, it follows that the parities of states of different charges cannot be compared.»

That understanding was achieved a decade later by Haag and Swieca as I will relate.

3. – The hypothesis of commuting superselection rules and Jauch's theorem; Wigner and Yanase's skew information.

In the course of the 1950's, some additional candidates for superselection rules were added to those mentioned in W[3], defined by the operators $(-1)^{2j}$ (univalence), Q (electric charge), and B (baryon number). The possibility that a lepton number exists and defines a superselection rule was discussed. On the other hand, a superselection rule (Bargmann's mass superselection rule) was derived for quantum theories invariant under the Galilei group [14]. Furthermore, it was recognized that in addition to the irreducible representations of the Poincaré group for which $U(i_t)^2 = (-1)^{2j}$, it is mathematically possible to construct irreducible representations for which $U(i_t)^2 = -(-1)^{2j}$ and that this distinction defines a superselection rule. An analogous argument can be made for space-time inversion i_{st} where $i_{st}\{t, \boldsymbol{x}\} = \{-t, -\boldsymbol{x}\}$, and so there are altogether four types of particles of given mass and spin. There is an associated superselection rule which Michel and I called the Type Superselection Rule [15, 16].

Ten years later the Type Superselection Rule was no longer of fundamental interest since experiment had shown that time inversion and space-time inversion are not exact symmetries of Nature. The surviving exact symmetry represented by an antiunitary operator was and is CPT.

The existence of CPT symmetry is, as is well known, a general theorem of local relativistic quantum field theory [17]. The proof constructs an anti-unitary operator, θ, which acts on a charged scalar field, ϕ, for example, as follows:

$$\theta^{-1}\phi(x)\theta = \phi^*(-x). \tag{3.1}$$

If the fields of the theory are tensors and spinors, then one can show that

$$\theta^2 = (-1)^{2j} \tag{3.2}$$

and the logical possibility

$$\theta^2 = -(-1)^{2j} \tag{3.3}$$

is excluded [18]. The distinction between (3.2) and (3.3), if both occurred in a quantum theory, would give rise to a surviving version of the Type Superselection Rule.

It was a striking feature of all these quantities defining candidates for superselection rules, even including the ones that have not survived, that they all commute so that one can diagonalize them simultaneously. Then the Hilbert space decomposes into a direct sum of coherent subspaces, in each of which all the superselected integrals of motion take definite values. That this tidy situation occurs in Nature was called the Hypothesis of Commuting Superselection Rules.

Now I want to quote a theorem by Jauch that relates this high-flying Hypothesis to a concept that is introduced in every first-year quantum mechanics course: the notion of a complete set of commuting observables. However, before I can state Jauch's result, I have to say a word about a change in the formalism of relativistic quantum theory that was taking place at the end of the 1950's. In an effort to bring the resources of algebra to bear on the general problems of the subject, people began to work with bounded observables and the algebras they generate rather than with unbounded field operators. (This can be regarded as the analogue of working with the bounded operator of multiplication by $\exp[-\alpha q^2]$ for $\alpha > 0$, a bounded operator, rather than with multiplication by q^2 an unbounded operator.) This choice of language makes it awkward to express the content of Lagrangian field theory, but it is natural for the discussion of superselection rules as we shall see.

Let $\mathscr{A}$ be the algebra generated by the bounded observables of a quantum theory. It is by definition the smallest algebra which contains all the bounded observables and all operators obtained from them by taking linear combinations, products and adjoints as well as suitably defined limits. An algebra closed under these operations is called a von Neumann algebra when the notion of limit is the so-called weak limit in which a sequence of operators A_i, $i = 1, 2, 3, \ldots$ converges when all matrix elements $(\phi, A_i\psi)$ converge for every pair of vectors ϕ, ψ in the Hilbert space, $\mathscr{H}$, of states. Then $\mathscr{A}'$, the commutant of $\mathscr{A}$, consists of all bounded operators in $\mathscr{H}$ that commute with every operator in $\mathscr{A}$. When, as is assumed here, $\mathscr{A}$ is the algebra generated by the observables, then $\mathscr{A}'$ is the algebra generated by the superselection rules. Now an algebra $\mathscr{B}$ is commutative if $\mathscr{B} \subset \mathscr{B}'$ and a von Neumann algebra, according to a basic theorem of von Neumann, satisfies $\mathscr{B} = (\mathscr{B}')'$. Thus, the Hypothesis of

Commutative Superselection Rules can be stated:

$$\mathcal{A}' \subset (\mathcal{A}')' = \mathcal{A} .$$

This condition can be restated in terms of the center, $\mathcal{Z}(\mathcal{A})$, of $\mathcal{A}$ which is defined as

$$\mathcal{Z}(\mathcal{A}) = \mathcal{A} \cap \mathcal{A}' .$$

The Hypothesis of Commutative Superselection Rules then says

$$\mathcal{Z}(\mathcal{A}) = \mathcal{A}' .$$

Now for the notion of a complete set of commuting observables. We interpret this phrase to mean a maximal commutative subalgebra of $\mathcal{A}$, *i.e.* a subalgebra $\mathcal{B}$ of $\mathcal{A}$ that is commutative

$$\mathcal{B} \subset \mathcal{B}'$$

and maximal in $\mathcal{A}$

$$\mathcal{B}' \cap \mathcal{A} \subset \mathcal{B} .$$

We then have

Theorem (Jauch [19]). The von Neumann algebra $\mathcal{A}$ generated by the observables contains a complete commuting set of observables if and only if the Hypothesis of Commutative Superselection Rules is satisfied. Then $\mathcal{Z}(\mathcal{A}) = \mathcal{A}'$.

Thus, the Hypothesis of Commutative Superselection Rules is not so outlandish. On the other hand, at the time there was no systematic rationale for the existence of the particular set of superselection rules that appeared to be present in Nature. Such a systematic theory came later with the work over several decades of Haag, Araki, Kastler, Doplicher, and Roberts as I will relate.

Another development at the end of the 1950's was the introduction by Wigner and Yanase of a quantity, the skew information, which in some sense measures how off-diagonal a state is relative to a self-adjoint operator [20]. Such a quantity can be used to characterize physical states in the presence of superselection rules: a physically realizable state will have zero skew information relative to an operator that defines a superselection rule. Suppose the state in question is defined by a density matrix, ρ, *i.e.* a positive operator of finite trace which we normalize to 1:

$$\operatorname{tr} \rho = 1 .$$

Then ρ has a uniquely determined positive square root $\rho^{1/2}$. Suppose the self-adjoint operator is A. Then the skew information of ρ relative to A is defined as

$$\mathcal{I}(\rho, A) = \frac{1}{2} \operatorname{tr}([A, \rho^{1/2}][\rho^{1/2}, A]) = \operatorname{tr}(\rho A^2) - \operatorname{tr}(A\rho^{1/2}A\rho^{1/2}) .$$

Wigner and Yanase showed that $\mathcal{I}(\rho, A)$:

a) is positive and vanishes for ρ a vector state, *i.e.* for ρ of rank one satisfying $\rho^2 = \rho$;

b) is invariant under the temporal evolution

$$A \to A_t = \exp[iHt] A \exp[-iHt],$$

$$\rho \to \rho_t = \exp[iHt] \rho \exp[-iHt];$$

c) is convex in ρ,

$$\mathscr{T}(a\rho_1 + (1-a)\rho_2) \leqslant a,\ \mathscr{T}(\rho_1, A) + (1-a)\ \mathscr{T}(\rho_2, A)$$

for $0 \leqslant a \leqslant 1$;

d) if $\rho = \rho_1 \otimes \rho_2$ and $A = A_1 \otimes \mathbf{1} + \mathbf{1} \otimes A_2$, then

$$\mathscr{T}(\rho_1 \otimes \rho_2, A_1 \otimes \mathbf{1} + \mathbf{1} \otimes A_2) = \mathscr{T}(\rho_1, A_1) + \mathscr{T}(\rho_2, A_2).$$

b) can be interpreted to mean that skew information does not decay as the state evolves in time. *c*) is characteristic not only of skew information but also of information defined as negative entropy. Thus, alternative definitions of skew information are possible, for example, as suggested by Dyson,

$$\mathscr{T}_\alpha(\rho, A) = \mathrm{tr}(\rho, A^2) - \mathrm{tr}(A\rho^\alpha A\rho^{(1-\alpha)})$$

for $0 < \alpha < 1$. This line of argument played an important role in the evolution of the theory and application of entropy in quantum statistical mechanics as one can read in the review article of Wehrl [21]. *d*) is important in the theory of measurement as developed by Wigner, Araki, and Yanase [22, 23] in which the composite system consisting of the measuring apparatus and the measured system is studied.

The importance of the skew information for the theory of superselection rules is that it gives a necessary condition for a state to be physically admissible in the presence of a superselection rule A: if ρ is to be physically admissible it must possess zero skew information relative to A.

4. – Quantum electrodynamics and the charge superselection rule.

In the mid 1960's Haag and Swieca found an argument which seemed to show that the charge superselection rule is a consequence of Gauss's Law for the electric charge density

$$\nabla \cdot \mathscr{E} = \rho. \tag{4.1}$$

(See [24] and the introduction of [25].) They noted that the charge in a sphere of radius R can be written:

$$Q_R = \int_{|\boldsymbol{x}| \leqslant R} \mathrm{d}^3x \rho(t, \boldsymbol{x}) = \int_{|\boldsymbol{x}| = R} \mathrm{d}\boldsymbol{S} \cdot \mathscr{E}(t, \boldsymbol{x}). \tag{4.2}$$

Now if A is an observable from a region inside the sphere of radius R and $\boldsymbol{x}$ lies on the sphere $|\boldsymbol{x}| = R$,

$$[A, \mathscr{E}(t, \boldsymbol{x})] = 0, \tag{4.3}$$

so

$$[A, Q_R] = \int_{|x|=R} \mathrm{d}\boldsymbol{S}\cdot[A, \mathcal{E}(t, \boldsymbol{x})] = 0 \tag{4.4}$$

and

$$[A, Q] = \lim_{R\to\infty} [A, Q_R] = 0\,. \tag{4.5}$$

I believe that this argument is essentially correct but that the proof is not. The objections come in two parts:

a) Gauss law (4.1) is not valid as an operator identity in local or covariant gauges.

b) In the Coulomb gauge where Gauss law is an operator identity, renormalization constants appear in (4.2), and the charge-carrying fields are not local so that there are difficulties in constructing the local observables.

These objections are overcome in [25] by a systematic use of a local gauge in the indefinite metric (Gupta-Bleuler) formulation of quantum electrodynamics. Thus, the charge superselection rule has to be regarded as a consequence of the laws of quantum electrodynamics.

5. – The Haag-Kastler quasi-local algebra and superselection rules.

In the decade that succeeded the introduction of the notion of superselection rule, the possibility that the algebra of observables of a quantum-mechanical theory might have a non-trivial center became familiar but, apart from the argument in W^3 that time inversion invariance implies the univalence superselection rule, there was no theory of superselection rules, no principles which would determine which particular set of superselection rules should occur in a particular theory. This situation was changed fundamentally in 1964 by the Haag-Kastler theory of local algebras of observables [26].

Haag and Kastler built several general ideas into their theory:

a) It should be based on the algebraic structure of the observables;

b) It should work with local observables, that is observables describing events in bounded regions of space-time;

c) The states of the theory should determine the representations that appear in the different superselection sectors.

a) can be regarded as a variation on a theme which appeared in the early days of quantum mechanics where the canonical commutation relations of the coordinates and moments generate an algebra which determines the structure of non-relativistic quantum mechanics. *b*) was surely influenced by experience in quantum field theory where the basic objects are operator-valued distributions. For example, the electric charge density, $\rho(x)$, has to be smeared with a smooth test function, f, on space-time to form $\int \mathrm{d}^4x f(x)\,\rho(\psi) = \rho(f)$ before one gets a well-defined operator in the Hilbert space of states. One can associate such an operator with a space-time region, $\mathcal{O}$, if the support of f, the region where it is nonvanishing, is contained in $\mathcal{O}$. One can think of the Haag-Kastler algebra of the region $\mathcal{O}$ as consisting of bounded functions of such observables as $\rho(f)$. c) is the key to the Haag-Kastler theory of superselection rules.

So Haag and Kastler assumed that for each bounded space-time region $\mathcal{O}$ there is an associated algebra $\mathcal{A}(\mathcal{O})$ and $\mathcal{O}_1 \subset \mathcal{O}_2$ implies $\mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O}_2)$. By taking the union over all $\mathcal{O}$ one gets the local algebra $\bigcup_{\mathcal{O}} \mathcal{A}(\mathcal{O})$. Now comes a key technical point. HK assumed their algebras $\mathcal{A}(\mathcal{O})$ are C^*-algebras. C^*-algebras have a norm $\| \ \|$ and are complete in the topology defined by the norm. The closure of $\bigcup_{\mathcal{O}} \mathcal{A}(\mathcal{O})$ in the norm is a C^*-algebra, $\mathcal{A}$, called the *quasi-local algebra*. Although the limit points in $\mathcal{A}$ may not belong to the $\mathcal{A}(\mathcal{O})$ of any particular bounded region $\mathcal{O}$, they can be regarded as «essentially» local.

To these geometrical assumptions HK added what they called Einstein causality (= local commutativity of observables):

$$\text{If } \mathcal{O}_1 \subset \mathcal{O}', \quad \text{then } \mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O})' .$$

Here $\mathcal{O}'$ is the space-like complement of $\mathcal{O}$, the set of all points y such that $y - x$ is space-like for every $x \in \mathcal{O}$.

This structure consisting of the quasi-local algebra, $\mathcal{A}$, and its family of local subalgebras, $\mathcal{A}(\mathcal{O})$, is referred to as a *net of local algebras*.

Now a word about C^*-algebras. What is a C^*-algebra? It is a Banach $*$-algebra satisfying the identity $\|A^*A\| = \|A\|^2$. That is, it is a set $\mathcal{A}$ with a definition of addition: $A, B \mapsto A + B \in \mathcal{A}$, and scalar multiplication: $A \to \alpha A$ (α, a complex number). That makes it a *vector space over the complex numbers*. It has an associative and distributive law of multiplication

$$A(BC) = (AB)C ,$$

$$A(B + C) = AB + BC ,$$

$$(\alpha A)B = A(\alpha B) = \alpha(AB) ;$$

that makes it an *associative algebra over the complex numbers*. It has a $*$-operation such that

$$(A^*)^* = A , \qquad (A + B)^* = A^* + B^* ,$$

$$(\alpha A)^* = \bar{\alpha} A^* , \qquad (AB)^* = B^* A^* ;$$

that makes it a $*$-*algebra*. It has a norm $\| \ \|$ satisfying

$$\|A + B\| \leqslant \|A\| + \|B\| ,$$

$$\|AB\| \leqslant \|A\| \, \|B\| ,$$

$$\|A^*\| = \|A\| ,$$

$$\|\alpha A\| = |\alpha| \, \|A\|$$

and it is complete in that norm; that makes it a *Banach* $*$-*algebra*. Finally, its norm satisfies $\|A^*\| = \|A\|^2$; that together with all the preceding makes it a C^*-*algebra*.

What is so good about C^*-algebras? First, every such algebra is isomorphic with preservation of norms to an algebra of operators in a Hilbert space with $*$ going over into the ordinary adjoint operation. So the abstract characterization of a C^*-algebra captures the concrete version exactly. This means that the representations of the quasi-local algebra, $\mathscr{A}$, occurring in the different superselection sectors can be isomorphic as C^*-algebras, even though they are not unitarily equivalent. Second, the representation theory of C^*-algebras is so extraordinarily well adapted to the purpose of local quantum field theory that it seems to be a case of pre-established harmony. This is a matter of such fundamental importance for the understanding of superselection rules that yet another mathematical excursion seems justified.

A *state* on a C^*-algebra, $\mathscr{A}$, is defined to be a positive linear form, ρ, on $\mathscr{A}$ that is normalized to 1 on the unit element, $\mathbf{1}$, of $\mathscr{A}$ (we assume it has one):

$$\begin{cases} \rho(\alpha A + \beta B) = \alpha\rho(A) + \beta\rho(B), \\ \rho(A^*A) \geqslant 0, \\ \rho(\mathbf{1}) = 1. \end{cases} \tag{5.1}$$

A $*$*-representation* of $\mathscr{A}$ in a Hilbert space $\mathscr{H}$ is a mapping, π, of $\mathscr{A}$ into $\mathscr{L}(\mathscr{H})$ the algebra of bounded linear operators in a Hilbert space $\mathscr{H}$ such that

$$\begin{cases} \pi(\alpha A + \beta B) = \alpha\pi(A) + \beta\pi(B), \\ \pi(AB) = \pi(A)\pi(B), \\ \pi(A^*) = [\pi(A)]^*. \end{cases} \tag{5.2}$$

The representation π is *cyclic* with cyclic vector ψ if the set of vectors $\{\pi(A)\psi;\ A \in \mathscr{A}\}$ is dense in $\mathscr{H}$. There is an intrinsic relation between the states of $\mathscr{A}$ and the cyclic representations of $\mathscr{A}$:

G(elfand) N(aimark) S(egal) *Construction*.

If ρ is a state on $\mathscr{A}$, there exists a cyclic representation π_ρ in a Hilbert space $\mathscr{H}_\rho$ with cyclic vector, ψ_ρ, such that

$$\rho(A) = (\psi_\rho, \pi_\rho(A)\psi_\rho). \tag{5.3}$$

Furthermore, if G: $g \mapsto \alpha_g$ is a representation of a group, G, by automorphisms of $\mathscr{A}$ and ρ is invariant under G in the sense that

$$\rho(\alpha_g(A)) = \rho(A), \tag{5.4}$$

then there exists a unitary representation of G: $g \mapsto U(g)$ such that

$$U(g)\pi_\rho(A)U(g)^{-1} = \pi_\rho(\alpha_g(A)) \tag{5.5}$$

and

$$U(g)\psi_\rho = \psi_\rho. \tag{5.6}$$

Thus, the theory of superselection rules can be reduced to the study of states on the quasi-local algebra.

The Haag-Kastler theory works in nonrelativistic theories as well as relativistic, but in relativistic theories it is natural to require that there exists a representation of the relativity group $G: g \mapsto \alpha_g$ by automorphisms of the quasi-local algebra $\mathcal{A}$ such that

$$\alpha_g(\mathcal{A}(\mathcal{O})) = \mathcal{A}(g(\mathcal{O})).$$

For G the Poincaré group an invariant state, ρ_0, then yields via the GNS construction a cyclic vector ψ_{ρ_0}, which we call ψ_0 for short, and a unitary representation of the Poincaré group, $\mathcal{P}_+^\uparrow$, $g \to U(g)$ such that

$$\pi(\alpha_g(A)) = U(g)\pi(A)U(g)^{-1}, \qquad g \in \mathcal{P}_+^\uparrow \tag{5.7}$$

and

$$U(g)\psi_0 = \psi_0, \qquad g \in \mathcal{P}_+^\uparrow, \tag{5.8}$$

i.e. ψ_0 (or its parent state ρ_0) is what is usually called a *vacuum state.*

The problem of determining which states give rise to physically acceptable representations is an important one in local quantum theory. For a theory invariant under the Poincaré group a natural condition is to require that for each state, ρ, there is a representation of the Poincaré group, $g \mapsto U_\rho(g)$, satisfying

$$\pi_\rho(\alpha_g(A)) = U_\rho(g)\pi_\rho(A)U_\rho(g)^{-1} \qquad \text{for all } A \in \mathcal{A}$$

and the *spectral condition*: the energy momentum operator associated with U_ρ has spectrum in the fore-cone: $\{p; p\cdot p \geq 0, p^0 \geq 0\}$. This restriction of ρ is usually referred to in Poincaré-invariant local quantum theory as the positive-energy condition. There are others such as Haag duality

$$\pi_\rho(A(\mathcal{O})) = \pi_\rho(\mathcal{A}(\mathcal{O}')') \tag{5.9}$$

but I will not go into that.

Instead, let me consider a slightly different question. Suppose one is given a vacuum state, ρ_0, of a local quantum theory. It defines a vacuum sector, $\mathcal{H}_{\rho_0}$. Are there other superselection sectors and, if so, how can one characterize the states that define them? This question was taken up in a grand investigation of Doplicher, Haag and Roberts [27] and brought to an even grander conclusion by Doplicher and Roberts [28]. Doplicher, Haag and Robert's criterion is based on the idea that superselection sectors other than the vacuum should be physically indistinguishable from the vacuum sector in the following very strict sense. Let A and B be any two points of space-time with B in the past cone whose vertex is at A. Let K be the region (double-cone) obtained by taking the intersection of the past cone with vertex at A and the future cone with vertex at B. If K' is the space-like complement of K, *i.e.* the set of all points space-like separated from every point of K, then a state ρ on the quasi-local algebra $\mathcal{A}$ satisfies:

The DHR *selection criterion.*

There exists a double cone K such that representation π_ρ restricted to K' is unitary equivalent to π_{ρ_0} restricted to K'. In formulae: given any such K there exists a unitary operator V mapping $\mathcal{H}_\rho$ onto $\mathcal{H}_{\rho_0}$ such that for all $A \in \mathcal{A}(K')$,

$$\pi_\rho(A) = V^{-1}\pi_{\rho_0}(A)V.$$

Doplicher, Haag and Roberts arrived at this criterion by starting with a theory in which the quasi-local algebra of observables, $\mathscr{A}$, is a subalgebra of a field algebra, $\mathscr{F}$, on which there acts a compact gauge group, G, and $\mathscr{A}$ consists precisely of those elements of $\mathscr{F}$ invariant under the action of the gauge group. Doplicher and Roberts showed the converse: every theory in which the superselection sectors are obtained by the DHR selection criterion can be obtained by the just mentioned DHR construction using a compact gauge group.

The DHR selection criterion was designed to work for theories with a mass gap above the vacuum and it was not expected to work in the quantum-electrodynamics of massive charged particles. For such cases Buchholz and Fredenhagen [29] introduced a weaker selection criterion and Buchholz [30] went on to make a detailed study of its application to quantum electrodynamics.

The BF *selection criterion.*

A state ρ on the quasi-local algebra of observables $\mathscr{A}$ satisfies the BF selection criterion if there exists a space-like cone, $\mathscr{S}$, such that for some unitary operator, V, mapping $\mathscr{H}_\rho$ onto $\mathscr{H}_{\rho^0}$,

$$\pi_\rho(A) = V^{-1}\pi_{\rho^0}(A)V \quad \text{for all } A \in \mathscr{A}(\mathscr{S}').$$

The set of superselection sectors is labeled by the unitary inequivalent representations π_ρ that satisfy the selection criterion. The detailed elaboration of the theory leads to particle and antiparticle structure and a treatment of their statistics based directly on the algebraic properties of observables [31, 32].

6. – Superselection rules induced by the environment; the shape of molecules.

As I have discussed, a superselection rule is associated with an operator that takes a definite value for every vector state of a quantum-mechanical system. The operator can therefore be regarded as a classical observable of the system. It is precisely this possibility that is exploited in the original Copenhagen interpretation of measurement in quantum mechanics. When a measurement of an observable, Q, of a system, S, is made using an apparatus, A, the wave function of the composite system $S + A$ evolves according to the Schrödinger equation in such a way that, for the resulting wave function, $\Psi_{S,A}$, the values of the observable, Q, of S are correlated with the readings of a macroscopic observable, the pointer, of A. The original Copenhagen interpretation of the act of measurement says that the wave function collapses to a mixture in which there is no interference between the different pointer readings. In the revised Copenhagen interpretation, recently summarized in [33], this collapse is interpreted as a process of decoherence arising from the interaction of the system S and the pointer with the rest of the degrees of freedom of the apparatus, A. The decoherence is complete and the standard prescription for computing the probability of a pointer reading is exact only in the limit in which the number of degrees of freedom of the apparatus is infinite.

The origins of this view of the implications of decoherence for the collapse of the wave function go back nearly half a century, but it is only in the last two decades that the full significance of it for the validity of classical macroscopic physics have begun to be explored [34, 35]. For a semipopular survey of the history see [36]. There are plenty of hard problems in quantum statistical mechanics still unsolved in this general territory, but I would like to devote the rest of this paper to a physically attractive case, the problem of the shape of molecules, and, in particular, of pyramidal molecules, like ammonia NH_3, phosphine PH_3, and arsine AsH_3.

What is at issue here is a clash between the conservation law of parity and the occurrence in Nature and in the laboratory of stable molecules that have a definite chirality [37]. Parity surely defines an integral of motion for the Hamiltonian which describes non-relativistic point electrons and nuclei interacting by Coulomb forces, and coupled to a transverse radiation field. Of course, this theoretical model omits the parity-violating weak interactions, and I will do so in all the following. More explicitly, a neutral molecule is composed of nuclei with position coordinates, $X_1, \ldots, X_k$ and charges $Z_1 e, \ldots, Z_k e$, respectively, as well as l electrons with position coordinates $x_1, \ldots, x_l$. Here $l = \sum_{j=1}^{k} Z_j$. For simplicity, the spin variables of nuclei and electrons are suppressed. A qualitative guide to the structure of the eigenstates of the Hamiltonian is provided by the first step in the Born-Oppenheimer approximation method: compute the energy, $E(X_1, \ldots, X_k)$, of the electrons with the nuclei held fixed at $X_1, \ldots, X_k$. If $E(X_1, \ldots, X_k)$ has a local minimum stationary value as a function of $X_1, \ldots, X_k$ for $X_j = Y_j$, $j = 1, \ldots, k$, and the corresponding wave function for the electrons is $\Psi_{Y_1, \ldots, Y_k}(x_1, \ldots, x_l)$, then $(U(I_s)\Psi)_{Y_1, \ldots, Y_k}(x_1, \ldots, x_l) = \Psi_{-Y_1, \ldots, -Y_k}(-x_1, \ldots, -x_l)$ also yields a local minimum stationary value and has the same energy. If $Y_1, \ldots, Y_k$ and $-Y_1, \ldots, -Y_k$ are different configurations of the nuclei, then the wave functions

$$\Psi^{(\pm)}_{Y_1, \ldots, Y_k}(x_1, \ldots, x_k) = \Psi_{Y_1, \ldots, Y_k}(x_1, \ldots, x_l) \pm \psi_{-Y_1, \ldots, Y_k}(-x_1, \ldots, -x_l)$$

have parity ± 1, respectively, under the action of the operator $U(I_S)$. The modern theory of the Schrödinger operator [37], tells us that there are exact eigenfunctions, $\Psi^{(\pm)}$, of the molecular Hamiltonian with the same qualitative features. The energy gap between the corresponding exact eigenvalues can be estimated by computing higher-order corrections in the Born-Oppenheimer method—it depends on the energy barrier separating $Y_1, \ldots, Y_k$ and $-Y_1, \ldots, -Y_k$ in the energy surface $E(X_1, \ldots, X_k)$. Pairs of states of this kind are customarily referred to as inversion doublets. The corresponding chiral states, $1/2\,(\Psi^{(\pm)} \pm \Psi^{(-1)})$, are, of course, not eigenstates of the molecular Hamiltonian.

So much for the behavior of a single molecule—could the environment persuade the molecule to become chiral? Might the inversion doublet collapse, suffering a kind of phase transition, and give rise to degenerate chiral states which if they were distinguishable could have an unobservable relative phase?

The first proposal for such a mechanism was made in the ETH-Zürich thesis of Pfeifer. He argued that the coupling of a single molecule to the soft photons of the electromagnetic field could give rise to such a phase transition. He modeled the system as a so-called spin-boson model in which all states of the molecule are ignored except those of a single inversion doublet, and a simplified version of the coupling to the radiation field is used. Calculating in mean-field approximation, he showed that the coupling to the boson field causes a phase transition to two degenerate chiral states, for sufficiently small splitting of the inversion doublet of the unperturbed molecule. Later on, a rigorous treatment showed that the phase diagram in the splitting *vs.* coupling-constant plane is a bit more complicated but for a large domain of splittings and coupling strengths the states of the system do form a degenerate pair of chiral states, and these states are disjoint in the sense that their relative phase is unobservable. However, it was also shown later that for any temperature $T > 0$, no such phase transition takes place. Thus, if the spin-boson model provides a reliable guide to the behavior of the predictions of the full Hamiltonian for the molecule coupled to the radiation field (now that is an example of a hard problem in quantum statistical mechanics for you), the Pfeifer mechanism cannot be responsible for the existence of isolated stable chiral molecules, except at $T = 0$. Rather than listing all the papers that provide the support for the statements of this paragraph, let me cite the rather complete review of Amann [38].

Shortly after Pfeifer proposed his mechanism, Jona-Lasinio, Martinelli and Scoppola [39] located an alternative mechanism which is based on the great sensitivity of delocalized eigenfunctions for symmetrical potentials and multiple minima to asymmetrical perturbations. Their work made possible a quantitative treatment of the effects of the environment on a molecule in an approximation in which the surrounding molecules are regarded as creating a perturbing potential [40]. The method was worked out in explicit detail by Claverie and Jona-Lasinio for three molecules: NH_3, PH_3, and AsH_3 [41]. When unperturbed, these molecules have a ground-state wave function invariant under reflection in the plane of the hydrogens. They have an excited state nearby which is odd under that reflection. Both these states are delocalized in the sense that the heavy nucleus has equal probabilities of being on the two sides of the plane of the hydrogens. However, a sufficiently large but still small repulsive perturbation potential acting on one side of the plane pushes the nuclei into a pyramidal configuration; the molecules have then acquired a definite shape.

Claverie and Jona-Lasinio argue that in the presence of an environment consisting of polarizable molecules, the pyramidal configuration is stabilized by the same mechanism that causes a dielectric to exhibit a macroscopic polarization density. They make detailed calculations for the three gases at room temperature and one atmosphere pressure and show that for arsine the mechanism produces a pyramidal configuration, while for ammonia the effective perturbation is not enough and the delocalized states survive. Phosphine is somewhere in between but ends up behaving like arsine. The predicted behavior for ammonia is in accord with what every microwave spectroscopist knows: the ammonia inversion line corresponding to the transition between the delocalized ground state and the above-mentioned odd delocalized excited state has been studied for fifty years. Pioneering theoretical work on the effect of the molecular environment on the inversion line was done in the Harvard thesis of Anderson [42]. He showed that the effect of collisions is to broaden and distort the line shape and to shift the line to the red [43]. A series of experiments on the absorption of microwaves in NH_3 and ND_3 as a function of frequency and pressure eventually led to the result that the level splitting decreases monotonically with increasing pressure becoming zero at 1.84 atmospheres for NH_3 and 0.125 atmospheres for ND_3 [44]. Presumably, above these pressures, NH_3 and ND_3 are gases of pyramidal molecules. These pyramidal molecules and PH_3 and AsH_3 are not chiral in Kelvin's sense because the three hydrogens are indistinguishable. However, a pyramidal molecule with four distinguishable nuclei is chiral and the chiral variable that distinguishes the two enantiomorphs may be chosen to be the orientation of the tetrahedron formed by the nuclei [45]. So far as I know, no one has had the patience and skill to make the two kinds of NHDT so far.

I find this story of the pyramidal molecules and the Jona-Lasinio, Martinelli, Scoppola mechanism quite convincing, but it seems to me that there are very challenging experimental and theoretical problems left. Even the definition of what one means by a superselection rule for a system induced by its environment has not been made sufficiently precise. Can the definition always be stated in terms of the density matrix of the system or does it involve the state of (system + environment)? How can the unobservability of relative phases predicted by such a superselection rule be given a clear-cut experimental test? I think that the 150 years long history of theory and experiment for the dielectric constant of a non-conductor and its relation to the electric moments of molecules is instructive as providing a perspective on these problems, but that is another long story and I am sure that I have already exhausted your patience.

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