

Zeitschrift: Helvetica Physica Acta
Band: 41 (1968)
Heft: 4

Artikel: On the asymptotic condition of scattering theory
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DOI: <https://doi.org/10.5169/seals-113902>

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On the Asymptotic Condition of Scattering Theory

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Abstract. A new and more general asymptotic condition for scattering systems is formulated. It is based on a physically motivated topology in the set of all states. This topology turns out to be the same as that induced by the trace norm. The existence of wave operators is demonstrated in this more general setting and the relation of these generalized wave operators to the conventional ones is clarified. A simple example is mentioned of a system which satisfies the new but not the old asymptotic condition.

1. Introduction

The purpose of this paper is to analyze the so-called *asymptotic condition* of scattering theory. This condition expresses the physically essential property of a scattering system, viz. that it behaves like a system of free particles in the remote past and in the distant future. The mathematically rigorous scattering theory dates from the time that this condition was first expressed in a mathematically rigorous form by one of the authors [2].

The problems which such a formulation must solve are: to give a physical motivation for the choice of a topology in the set of the states of the system; to formulate the asymptotic condition in this topology; and to render explicit its consequences.

The previously used definition of the asymptotic condition *did* specify a topology and *did* furnish a starting point for scattering theory which is mathematically completely satisfactory. However, the physical motivation for this topology was not sufficient. Indeed certain rather trivial cases, which one could hardly exclude on physical grounds, are in fact excluded by the asymptotic condition of Reference [2]. For example, such a case is the one characterized by two evolution operators H_0 and $H = H_0 + c I$, where $c I$ is a real-valued constant times the identity operator.

For these reasons we reexamine here the asymptotic condition, keeping in mind the physical motivation for the choice of topology in the state space. This space is the set of all density operators W , that is, the set of all positive, self-adjoint operators in Hilbert space with trace 1. These operators are a subset of the linear space of all nuclear operators (sometimes also called traceclass operators). The nuclear operators are all those operators which admit a finite trace norm (to be defined below). We shall show in this paper that the topology induced by the trace norm is the natural topology which admits a simple physical interpretation.

We then examine the question to what extent the new asymptotic condition determines the Møller wave-operators and the scattering operators. We shall prove that the new asymptotic condition defines generalized wave operators and scattering operators, and we examine and clarify the nature of this generalization.

2. Mathematical Preliminaries

Throughout this paper we shall be concerned with a separable Hilbert space \mathcal{H} over the complex scalars. Of particular importance is the *trace class* of linear operators (cf. [1], [4], or [5]). If T is a compact operator which maps \mathcal{H} into \mathcal{H} , then T has the form $T = U |T|$ where $|T| = \sqrt{T^* T}$ is a positive-definite compact operator in \mathcal{H} , and U is an isometric operator which maps the range of T into \mathcal{H} [1, p. 29]. If $\lambda_1, \lambda_2, \dots$ are the non-negative eigenvalues of the operator $|T|$, then the *trace norm* of T is defined by

$$\|T\|_1 = \sum_{k=1}^{\infty} \lambda_k = \text{Tr } |T|. \quad (1)$$

The set of all T with $\|T\|_1 < \infty$ is the nuclear space $\mathcal{B}_1(\mathcal{H})$. Since the convergence of the series $\sum \lambda_k$ implies the convergence of the series $\sum \lambda_k^2$, the nuclear operators form a subclass of the Hilbert-Schmidt operators $\mathcal{B}_2(\mathcal{H})$.

We summarize some of the properties of nuclear operators [1], [4], or [5]:

- (a) $\mathcal{B}_1(\mathcal{H})$ is a noncommutative Banach *-algebra with the norm $\|\cdot\|_1$.
- (b) The product ST of any two Hilbert-Schmidt operators is a nuclear operator, and, conversely, every nuclear operator is the product of two Hilbert-Schmidt operators.
- (c) $\|T\|_1 = \|T^*\|_1 = \||T|\|_1$.
- (d) $|\text{Tr } T| \leq \|T\|_1$.
- (e) $\text{Tr } (S + T) = \text{Tr } S + \text{Tr } T$ and $\text{Tr } ST = \text{Tr } TS$.
- (f) $\|UT\|_1 = \|TU\|_1 = \|T\|_1$ for any unitary operator U .
- (g) $\|T\| \leq \|T\|_1$.
- (h) If $T \in \mathcal{B}_1(\mathcal{H})$ and $S \in \mathcal{B}(\mathcal{H})$ (the bounded operators), then

$$\|ST\|_1 \leq \|S\| \cdot \|T\|_1 \text{ and } \|TS\|_1 \leq \|T\|_1 \cdot \|S\|.$$

- (i) If $T \in \mathcal{B}_1(\mathcal{H})$ is symmetric, $\|T\|_1$ is equal to the sum of the absolute values of the repeated eigenvalues of T .

For convenience in terminology we define a *ray* to be a projection with one-dimensional range, i.e. $P^2 = P^* = P$ and $\|P\|_1 = \dim P = 1$.

Lemma 1

If E and F are rays, say $E = (\phi, \cdot) \phi$ and $F = (\psi, \cdot) \psi$, then

$$\|E - F\|_1 = 2 (1 - |(\phi, \psi)|^2)^{1/2} = 2 (1 - \|EFE\|_1)^{1/2}$$

and

$$\|E - F\| = 1/2 \|E - F\|_1 = (1 - \|EFE\|_1)^{1/2}.$$

Proof

By property (i) above $\|E - F\|_1$ is equal to the sum of the absolute values of the repeated eigenvalues of $(E - F)$. Furthermore, $\|E - F\|$ is equal to the magnitude of the maximum eigenvalue of $(E - F)$. Therefore, we calculate these eigenvalues.

Letting $g = (E - F)f$ in $(E - F)g = (\phi, g)\phi - (\psi, g)\psi$, we obtain

$$(E - F)^2 f = [(\phi, f) - (\psi, f)(\phi, \psi)]\phi - [(\phi, f)(\psi, \phi) - (\psi, f)]\psi.$$

Now equate $(E - F)^2 f$ to $\lambda^2 f$, let $f = \alpha\phi + \beta\psi$, and equate the coefficients of ϕ and ψ to obtain

$$\lambda^2 = 1 - |(\phi, \psi)|^2.$$

Thus the eigenvalues of $(E - F)$ are $\pm (1 - |(\phi, \psi)|^2)^{1/2}$. It follows that $\|E - F\| = (1 - |(\phi, \psi)|^2)^{1/2} = (1 - \|EF\|^2)^{1/2}$, and $\|E - F\|_1 = 2(1 - |(\phi, \psi)|^2)^{1/2} = 2(1 - \text{Tr } EFE)^{1/2} = 2(1 - \|EFE\|_1)^{1/2}$, q.e.d.

3. Topology in State Space

The essential property of a scattering system is that the actual time-evolution of the states of a scattering system becomes nearly indistinguishable from the time-evolution of the free particle states in the remote past and in the distant future. We shall now transcribe this property into appropriate mathematical language. The main problem is to give precise meaning to the heuristic expression 'nearly indistinguishable'.

The expression clearly refers to an *asymptotic limiting property*. If such a property is to be made precise, we need a topology in the set $\mathcal{W}(\mathcal{H})$ of all the states. This set consists of all density operators W on \mathcal{H} , i.e., all W for which $W^* = W \geq 0$ and $\text{Tr } W = 1$.

The topology in a set is determined if the class of open sets is specified. A standard way to define the open sets is to give a family of neighborhoods which generate the open sets through the processes of unions and intersections. In the present context the neighborhoods can be defined through a numerical valued distance function which measures in terms of real numbers the distance between two states. How this distance function is defined depends on the physical interpretation of the limiting processes we wish to express.

The distance between two states must be a quantity which manifests itself through the expectation values of observables. Roughly speaking: Two states are close to each other if all the expectation values of observables are close to each other. If A is an observable and $W_1, W_2 \in \mathcal{W}(\mathcal{H})$ are two states, we may write for this difference

$$\langle A \rangle_1 - \langle A \rangle_2 = \text{Tr}(W_1 A) - \text{Tr}(W_2 A) = \text{Tr}(W_1 - W_2) A. \quad (2)$$

This quantity is, however, not yet suitable for defining a distance function in state-space. The fact that it is indefinite is relatively easily corrected by replacing it by the absolute magnitude. More disturbing is the fact that it is unbounded. Indeed if A is an observable, then λA with λ real is one too, and the substitution of A by λA multiplies the above expression by a factor λ . Thus, it is justified to admit only *normalized* observables. This we do by restricting ourselves to bounded observables with bound 1. Another difficulty stems from the fact that in general the set of all (bounded) observables is mathematically an ill-defined concept since its extent depends essentially on the skill of the experimenter. In order to obtain a mathematically more suitable set of operators we shall admit for A all operators of bound 1.

Further, in order to assure that no measurement whatsoever distinguishes two neighboring states to an arbitrary predetermined degree of precision, we need to require a *uniform* approximation with respect to all operators A .

With these motivations in mind we are led to consider the following functional on pairs of states

$$\varrho(W_1, W_2) \equiv \sup_{\|A\|=1} | \text{Tr} (W_1 - W_2) A |, \quad (3)$$

where the supremum is taken with respect to all operators of norm 1. This distance function is in fact a *metric*, and the space $\mathcal{W}(\mathcal{H})$ of all states W is a *metric space*, i.e., the mapping of $\mathcal{W}(\mathcal{H}) \times \mathcal{W}(\mathcal{H})$ into the real numbers \mathcal{R} satisfies:

- (i) $\varrho(W, W) = 0$ and $\varrho(W_1, W_2) > 0$ if $W_1 \neq W_2$,
- (ii) $\varrho(W_1, W_2) = \varrho(W_2, W_1)$,
- (iii) $\varrho(W_1, W_3) \leq \varrho(W_1, W_2) + \varrho(W_2, W_3)$.

The choice of this topology which we have introduced in the state space $\mathcal{W}(\mathcal{H})$ was motivated by the proximity of the observable quantities for neighboring states. There is however a slight blemish in this formulation since we have had to introduce the supremum over all bounded operators of bound 1, and not just the observables (that is, the self-adjoint operators). This goes beyond the original intention and was done primarily for mathematical convenience.

The most satisfactory topology would have been the one generated with a distance function with the supremum taken over bounded self-adjoint operators only, or better still, projections. The projections are indeed the most important observables. They represent the so-called yes-no experiments and every other quantum mechanical observable (even unbounded) can be constructed from them via the spectral theorem [3, sec. 8-5]. For this reason we shall also define the metric

$$\varrho_0(W_1, W_2) \equiv \sup_{E^2=E=E^*} | \text{Tr} (W_1 - W_2) E |. \quad (4)$$

Of course it is hardly to be expected that the metric ϱ_0 defined with such a restricted class of operators should be identical with the metric ϱ which is defined for all bounded operators. However, it is not the distance function itself which is of primary interest but the asymptotic convergence properties based on the neighborhoods, defined with such functions. We shall show in the next section that ϱ and ϱ_0 imply the same asymptotic convergence properties.

We note that the right side of Equation (3) is meaningful for a larger class of operators than $\mathcal{W}(\mathcal{H})$. In fact, we shall prove:

Theorem 1

For any pair S, T of nuclear operators

$$\varrho(S, T) = \|S - T\|_1.$$

Proof

Using property (d) and then (h) we obtain

$$| \text{Tr} TA | \leq \|TA\|_1 \leq \|T\|_1 \|A\| = \|T\|_1.$$

Thus,

$$\varrho(T, O) = \sup_{\|A\|=1} |Tr TA| \leq \|T\|_1.$$

If $T \in \mathcal{B}_1(\mathcal{H})$, then T has a polar decomposition $T = U|T|$ where $|T| = \sqrt{T^*T}$ and U is an isometric operator which maps the range of $|T|$ into \mathcal{H} . Using the fact that U^*U is the identity operator on the range of $|T|$, and property (e), we obtain

$$\|T\|_1 = Tr|T| = Tr U^* U |T| = Tr U |T| U^* = Tr TU^* \leq \varrho(T, O).$$

It follows that

$$\varrho(T, O) = \|T\|_1 \text{ for all } T \in \mathcal{B}_1(\mathcal{H}),$$

or

$$\varrho(S, T) = \varrho(S - T, O) = \|S - T\|_1 \text{ for all } S, T \in \mathcal{B}_1(\mathcal{H}), \text{ q.e.d.}$$

Corollary

The metric space $\mathcal{W}(\mathcal{H})$ is a *closed convex* subset of the Banach space $\mathcal{B}_1(\mathcal{H})$ and hence is *complete*.

Proof

Suppose that $W_1, W_2 \in \mathcal{W}(\mathcal{H})$ and $0 \leq a \leq 1$. Define $W \equiv a W_1 + (1 - a) W_2$. Then

$$W^* = a W_1^* + (1 - a) W_2^* = a W_1 + (1 - a) W_2 = W,$$

and

$$Tr W = Tr a W_1 + Tr (1 - a) W_2 = a + (1 - a) = 1.$$

Hence $W \in \mathcal{W}(\mathcal{H})$ and $\mathcal{W}(\mathcal{H})$ is convex.

Suppose further that $W_n \in \mathcal{W}(\mathcal{H})$ is a sequence of density operators converging to a limit point $W \in \mathcal{B}_1(\mathcal{H})$, i.e., $\varrho(W_n, W) \rightarrow 0$ as $n \rightarrow \infty$.

By properties (e) and (d)

$$|1 - Tr W| = |Tr W_n - Tr W| = |Tr (W_n - W)| \leq \|W_n - W\|_1 \rightarrow 0$$

as $n \rightarrow \infty$. Therefore, $Tr W = 1$. Further, by the Cauchy-Schwartz' inequality and property (g), we have for all unit vectors $\theta, \phi \in \mathcal{H}$

$$\begin{aligned} |(W\theta, \phi) - (\theta, W\phi)| &\leq |(W\theta, \phi) - (W_n\theta, \phi)| + |(\theta, W_n\phi) - (\theta, W\phi)| \\ &\leq \|(W - W_n)\theta\| \cdot \|\phi\| + \|\theta\| \cdot \|(W_n - W)\phi\| \\ &\leq 2 \|W_n - W\| \leq 2 \|W_n - W\|_1 \rightarrow 0 \end{aligned}$$

as $n \rightarrow \infty$. Thus $(W\theta, \phi) = (\theta, W\phi)$, i.e., $W^* = W$. Positivity of W can also be as easily proved. Consequently, $W \in \mathcal{W}(\mathcal{H})$, and $\mathcal{W}(\mathcal{H})$ is closed, q.e.d.

It follows that the metric ϱ on $\mathcal{W}(\mathcal{H})$ may be extended to all $\mathcal{B}_1(\mathcal{H})$, where it is in fact a norm. This result is particularly useful because it enables us to express physically-motivated convergence properties in terms of the trace-norm topology, about which many theorems are known.

4. The Asymptotic Condition

In the preceding section we have introduced a physically-motivated topology in the state space $\mathcal{W}(\mathcal{H})$. Equipped with this topology we are now in a position to formulate the asymptotic condition for scattering systems. This condition must express the characteristic property of a scattering system, which is that the system evolves in the remote past and in the distant future like a system of free particles.

Let H_0 denote the evolution operator for a free particle and denote by H the evolution operator for the scattering system. Further, let $U_t = e^{-iH_0 t}$, $V_t = e^{-iH t}$, and if $W \in \mathcal{W}(\mathcal{H})$ is any state, let $\overset{\circ}{W}_t \equiv U_t W U_t^*$ and $W_t \equiv V_t W V_t^*$.

We shall say that H satisfies the *asymptotic condition* (A) if for every state $W \in \mathcal{W}(\mathcal{H})$ there exists a pair of states W^\pm (unique) such that:

$$(A): \quad \varrho(\overset{\circ}{W}_t, W_t^\pm) = \|\overset{\circ}{W}_t - W_t^\pm\|_1 \rightarrow 0 \text{ as } t \rightarrow \mp \infty.$$

It is clear that the condition (A) is a restriction on H since H_0 is given explicitly as the evolution operator of a free particle. Furthermore the condition (A) translates the physical characteristics of a simple, non-relativistic scattering system into precise mathematical language. The condition (A) is thus the point of departure of the entire scattering theory. A main objective of this theory is to extract the physically observable quantities from condition (A) and to relate them to the properties of the evolution operator H .

By property (f) we can transform (A) as follows:

$$\|\overset{\circ}{W}_t - W_t^\pm\|_1 \equiv \|U_t W U_t^* - V_t W^\pm V_t^*\|_1 = \|X_t W X_t^* - W^\pm\|_1$$

where $X_t = V_t^* U_t$. Thus (A) is equivalent to

$$(A): \quad \|X_t W X_t^* - W^\pm\|_1 \rightarrow 0 \text{ as } t \rightarrow \mp \infty.$$

We shall write for the above relation

$$W^\pm = \text{tr} - \lim_{t \rightarrow \mp \infty} X_t W X_t^* \quad (5)$$

and refer to W^\pm as the *trace-limit* of $W(t) \equiv X_t W X_t^*$.

The two limits $t \rightarrow \pm \infty$ have very similar properties and most of the theorems derived below are identical in wording for the two cases. Thus to simplify the notation we shall omit in the following the double index \pm and replace it by a prime. Furthermore we shall omit the designation $t \rightarrow \mp \infty$ which may be replaced at its proper place together with the double index at the end of any of the formulae to be derived in the following, to yield a correct and complete formula.

In this simplified notation the formula (5), for example, appears as

$$W' \equiv \mu(W) = \text{tr} - \lim X_t W X_t^* = \text{tr} - \lim W(t). \quad (6)$$

The mapping μ is thus defined on $\mathcal{W}(\mathcal{H})$ and maps $\mathcal{W}(\mathcal{H})$ into $\mathcal{W}(\mathcal{H})$. We now show that the correspondence $W \rightarrow W'$ maps pure states into pure states.

Lemma 2

If W is pure ($W^2 = W$), then W' is pure also.

Proof

Since $W^2 = W$, it follows that $W(t)^2 = X_t W^2 X_t^* = W(t)$, i.e., $W(t)$ is also pure for all t . Now

$$\begin{aligned} \|W'^2 - W'\|_1 &\leq \|W'^2 - W(t)^2\|_1 + \|W(t)^2 - W'\|_1 \\ &= \|[W' - W(t)] \frac{W' + W(t)}{2} + \frac{W' + W(t)}{2} [W' - W(t)]\|_1 + \|W(t) - W'\|_1 \\ &\leq 2 \|W' - W(t)\|_1 \left\| \frac{W' + W(t)}{2} \right\|_1 + \|W(t) - W'\|_1 \\ &= 3 \|W(t) - W'\|_1. \end{aligned}$$

Here we have used $\|W' + W(t)/2\|_1 = 1$ which is true since $\bar{W} \equiv 1/2 (W' + W(t)) \in \mathcal{W}(\mathcal{H})$ and hence $\|\bar{W}\|_1 = \text{Tr } \bar{W} \equiv 1$. Since $\|W(t) - W'\|_1$ tends to zero by condition (A), we have $\|W'^2 - W'\|_1 = 0$. This implies that $W'^2 = W'$, or that W' is pure, which proves the lemma.

Let us now investigate the effect on the asymptotic condition if we had chosen the distance function ϱ_0 or the operator norm as the metric on $\mathcal{W}(\mathcal{H})$ instead of $\varrho = \|\cdot\|_1$. We shall say that the evolution operator H satisfies the *asymptotic condition* (A_0) or (A') , respectively, if for every state $W \in \mathcal{W}(\mathcal{H})$ there exists a pair of states W^\pm (unique) such that:

$$(A_0) \quad \varrho_0(\overset{\circ}{W}_t, W_t^\pm) \rightarrow 0 \text{ as } t \rightarrow \mp \infty.$$

$$(A') \quad \|\overset{\circ}{W}_t - W_t^\pm\| = \|W(t) - W^\pm\| \rightarrow 0 \text{ as } t \rightarrow \mp \infty.$$

Theorem 2 The three asymptotic conditions (A), (A_0) , and (A') are all equivalent.

Proof We note that

$$\varrho_0(W_1, W_2) \equiv \sup_{E^2=E=E^*} |\text{Tr } (W_1 - W_2) E| \leq \sup_{\|A\|=1} |\text{Tr } (W_1 - W_2) A| = \|W_1 - W_2\|_1$$

by Theorem 1. On the other hand, if we take the supremum only over those projections $P^2 = P^* = P$ whose range has dimension 1, say $P\phi = \phi$, we observe

$$\varrho_0(W_1, W_2) \geq \sup_{\substack{P^2=P^*=P \\ \dim P=1}} |\text{Tr } (W_1 - W_2) P| = \sup_{\|\phi\|=1} |(\phi, (W_1 - W_2) \phi)| = \|W_1 - W_2\|.$$

Therefore, $\|W_1 - W_2\| < \varrho_0(W_1, W_2) < \|W_1 - W_2\|_1$.

It follows that $(A) \Rightarrow (A_0) \Rightarrow (A')$. It remains only to prove that $(A') \Rightarrow (A)$.

If P_1 and P_2 are two rays (projections with one-dimensional range), then by Lemma 1

$$\|P_1 - P_2\|_1 = 2 \|P_1 - P_2\|.$$

Furthermore, if W is a pure state and $\|W' - W(t)\| \rightarrow 0$ then W' (recall that $W' = W^\pm$) is pure too (proof is similar to the proof of Lemma 2). Hence for pure states

$$\|W' - W(t)\| \rightarrow 0 \text{ implies } \|W' - W(t)\|_1 \rightarrow 0.$$

Next let W be an arbitrary state and λ_r the positive (possibly repeated) eigenvalues of W arranged in descending order so that

$$W = \sum_r \lambda_r P_r \quad \sum_r \lambda_r = 1.$$

Then

$$W(t) = \sum_r \lambda_r P_r(t), \quad \text{where } P_r(t) = X_t P_r X_t^*.$$

Because of condition (A') all the $P_r(t)$ tend in the norm to some limit P'_r , and thus

$$W' = \sum_r \lambda_r P'_r.$$

We may thus write

$$W' - W(t) = \sum_r \lambda_r (P'_r - P_r(t))$$

and therefore

$$\|W' - W(t)\|_1 \leq \sum_r \lambda_r \|P'_r - P_r(t)\|_1 = 2 \sum_r \lambda_r \|P'_r - P_r(t)\|. \quad (7)$$

Now for any two rays P_1, P_2 we have by Lemma 1 $\|P_1 - P_2\| = \sqrt{1 - |(\phi_1, \phi_2)|^2}$, where ϕ_1 is a unit vector in the range of P_1 and ϕ_2 a unit vector in the range of P_2 . Hence $\|P_1 - P_2\| \leq 1$.

Considering now the sum at the right of Equation (7) we can divide it into two parts

$$\sum_{r=1}^{\infty} = \sum_{r=1}^N + \sum_{r=N+1}^{\infty}.$$

For the second part we choose N so large that

$$\sum_{r=N+1}^{\infty} \lambda_r \|P'_r - P_r(t)\| \leq \sum_{r=N+1}^{\infty} \lambda_r < \varepsilon/4.$$

For the first part we choose a τ so large that for all $t > \tau$ and all $r \leq N$ we have $\|P'_r - P_r(t)\| < \varepsilon/4$. With this choice we find

$$\|W' - W(t)\|_1 < \varepsilon/2 \sum_{r=1}^N \lambda_r + \varepsilon/2 < \varepsilon.$$

Since ε is arbitrary the left side tends to zero. This finishes the proof of Theorem 2.

The condition (A_0) is the closest mathematical transcription of the physical content of the asymptotic condition. The equivalence of (A_0) with the other two formulations is thus a very satisfactory result. Throughout the remainder of this paper we shall restrict ourselves to the asymptotic condition (A).

5. Consequences of the Asymptotic Condition

Equation (6) defines a mapping μ of $\mathcal{W}(\mathcal{H})$ into $\mathcal{W}(\mathcal{H})$. We now show that this mapping can be extended to $\mathcal{B}_1(\mathcal{H})$. First, we note that any $A \in \mathcal{B}_1(\mathcal{H})$ may be written as $A = A_1 + i A_2$ where $A_1 = 1/2 (A + A^*)$ and $A_2 = 1/(2i) (A - A^*)$ are self-adjoint. Second, any self-adjoint nuclear operator A_i ($i = 1, 2$) may be written as $A_i = A_i^+ - A_i^-$

where $A_i^\pm \geq 0$. For this we take $|A_i| = (A_i^2)^{1/2}$, and $A_i^\pm = 1/2 (|A_i| \pm A_i)$ ($i = 1, 2$). Finally, if $A_i^\pm > 0$, define $\lambda_i^\pm \equiv \text{Tr } A_i^\pm \neq 0$. Then $A_i^\pm = \lambda_i^\pm W_i^\pm$ where $W_i^\pm = (\lambda_i^\pm)^{-1} A_i^\pm \in \mathcal{W}(\mathcal{H})$. Therefore, we define $\mu(0) = 0$, $\mu(A_i^\pm) = \lambda_i^\pm \mu(W_i^\pm)$, $\mu(A_i) = \mu(A_i^+) - \mu(A_i^-)$ ($i = 1, 2$), and $\mu(A) = \mu(A_1) = i \mu(A_2)$. Note that with this construction every $A \in \mathcal{B}_1(\mathcal{H})$ is the linear combination of at most four states.

It follows that

$$\mu(A) \equiv \text{tr} - \lim X_t A X_t^* \equiv \text{tr} - \lim A(t), \quad (8)$$

$A(t) = X_t A X_t^*$, is a mapping from $\mathcal{B}_1(\mathcal{H})$ into $\mathcal{B}_1(\mathcal{H})$. Recall that the trace-limit is the limit in trace-norm as $t \rightarrow \mp \infty$, and we omit the designation $t \rightarrow \mp \infty$ since the two cases are entirely analogous.

Lemma 3 The mapping $\mu(A)$ has the following properties:

- (i) $\|\mu(A)\|_1 = \|A\|_1$
- (ii) $\mu(\alpha_1 A_1 + \alpha_2 A_2) = \alpha_1 \mu(A_1) + \alpha_2 \mu(A_2)$
- (iii) $\mu(A_1 A_2) = \mu(A_1) \mu(A_2)$
- (iv) $\mu(A^*) = \mu(A)^*$

Proof We indicate the method of proof by proving (iii). The other proofs are similar. Since $(A_1 A_2)(t) = A_1(t) A_2(t)$, property (iii) follows by taking the trace-limit of

$$\begin{aligned} \|\mu(A_1 A_2) - \mu(A_1) \mu(A_2)\|_1 &\leq \|\mu(A_1 A_2) - (A_1 A_2)(t)\|_1 \\ &\quad + \|A_1(t) [A_2(t) - \mu(A_2)]\|_1 + \|[A_1(t) - \mu(A_1)] \mu(A_2)\|_1. \end{aligned}$$

Corollary 1 The mapping μ is continuous with respect to the trace-norm topology.

Corollary 2 The mapping μ maps pure states into pure states.

Proofs By properties (ii) and (i)

$$\|\mu(A) - \mu(A_n)\|_1 = \|\mu(A - A_n)\|_1 = \|A - A_n\|_1,$$

hence, Corollary 1. Corollary 2 follows from properties (i), (iii), and (iv) since $\mu(W)^2 = \mu(W^2) = \mu(W) = \mu(W)^*$ if $W^2 = W = W^*$, and $\|\mu(P)\|_1 = 1$ if $\|P\|_1 = \dim P = 1$.

We note that if Ω is any isometry of Hilbert space, then the mapping $A \rightarrow \Omega A \Omega^*$ has all the properties (i) – (iv) of Lemma 3. The following theorem establishes the converse.

Theorem 3 Let $A \rightarrow \mu(A)$ be a mapping of the Banach algebra $\mathcal{B}_1(\mathcal{H})$ into $\mathcal{B}_1(\mathcal{H})$ which satisfies (i) – (iv). Then there exists an isometry Ω such that $\mu(A) = \Omega A \Omega^*$. Furthermore, the projection $F = \Omega \Omega^*$ reduces all the operators $\mu(A)$ and it is the smallest projection with this property.

Proof Any $A \in \mathcal{B}_1(\mathcal{H})$ has a canonical expansion or polar representation of the form

$$A = \sum_{k=1}^{\infty} \lambda_k(\psi_k, \cdot) \phi_k \quad (9)$$

with $\|A\|_1 = \sum \lambda_k < \infty$ (cf. [4] or [5]). Here $\{\phi_k\}$ and $\{\psi_k\}$ are orthonormal sequences, and the λ_k 's are the positive eigenvalues of $\sqrt{A^* A}$.

By Corollary 2 of Lemma 3, if P is a ray, then $\mu(P)$ is also a ray. For any unit vector $\phi \in \mathcal{H}$, $P = (\phi, \cdot) \phi$ is the ray such that $P \phi = \phi$. Since $Q \equiv \mu(P)$ is also a ray, there exists an $\omega \in \mathcal{H}$ such that $Q = (\omega, \cdot) \omega$. Thus the mapping μ associates an element $\omega \in \mathcal{H}$ with every $\phi \in \mathcal{H}$. The unit vector ω is unique up to a phase factor (a scalar multiple of modulus 1).

Now select some fixed $\phi_0 \in \mathcal{H}$ and decide on the phase factor for the corresponding ω_0 . If ϕ is any unit vector of \mathcal{H} , define $A_0 \equiv (\phi_0, \cdot) \phi$. Then $A_0^* = (\phi, \cdot) \phi_0$. Also,

$$A_0^* A_0 = (\phi, (\phi_0, \cdot) \phi) \phi_0 = P_{\phi_0},$$

and

$$A_0 A_0^* = (\phi_0, (\phi, \cdot) \phi_0) \phi = P_\phi.$$

Therefore, by properties (iii) and (iv)

$$\mu(A_0)^* \mu(A_0) = \mu(A_0^* A_0) = \mu(P_{\phi_0}) = Q_{\omega_0},$$

and

$$\mu(A_0) \mu(A_0)^* = \mu(A_0 A_0^*) = \mu(P_\phi) = Q_\omega.$$

It follows that $\mu(A_0)$ is an operator which maps the one-dimensional space $\{\omega_0\}$ into the one-dimensional space $\{\omega\}$. It may be written in the form $\mu(A_0) = \alpha (\omega_0, \cdot) \omega$, where α is a complex constant of modulus 1.

We now keep ϕ_0 and ω_0 fixed, and for each unit vector $\phi \in \mathcal{H}$ we choose the phase factor for the corresponding ω in such a way that $\alpha = 1$. Then

$$\mu(A_0) = (\omega_0, \cdot) \omega \text{ for all } \phi \in \mathcal{H}. \quad (10)$$

For any unit vectors $\phi_i, \phi_j \in \mathcal{H}$ define

$$A_{ij} \equiv (\phi_j, \cdot) \phi_i, \quad i, j = 0, 1, 2.$$

Then

$$A_{12} = (\phi_2, \cdot) \phi_1 = (\phi_0, (\phi_2, \cdot) \phi_0) \phi_1 = A_{10} A_{02}. \quad (11)$$

By property (iii) and Equation (10)

$$\mu(A_{12}) = \mu(A_{10}) \mu(A_{02}) = (\omega_0, (\omega_2, \cdot) \omega_0) \omega_1 = (\omega_2, \cdot) \omega_1. \quad (12)$$

Thus, the choice of the phase factors for ω_1 and ω_2 (with respect to the fixed ω_0) produces the mapping:

$$(\phi_2, \cdot) \phi_1 \rightarrow (\omega_2, \cdot) \omega_1 \text{ for all } \phi_1, \phi_2 \in \mathcal{H}.$$

Furthermore, if γ is any complex number of modulus 1, let $\phi \equiv \phi_1 + \gamma \phi_2$, and $A \equiv (\phi, \cdot) \phi$. Then by property (ii)

$$\mu(A) = \mu(P_{\phi_1} + P_{\phi_2} + 2 \operatorname{Re} \bar{\gamma} A_{12}) = Q_{\omega_1} + Q_{\omega_2} + 2 \operatorname{Re} \bar{\gamma} \mu(A_{12}) = (\omega, \cdot) \omega \quad (13)$$

where $\omega \equiv \omega_1 + \gamma \omega_2$. Now $\|A\|_1 = \|\phi\|^2$ ([5], p. 41), so that property (i) gives

$$\|\phi_1 + \gamma \phi_2\|^2 = \|A\|_1 = \|\mu(A)\|_1 = \|\omega_1 + \gamma \omega_2\|^2. \quad (14)$$

Expanding the squares in the left and right sides of this equation and simplifying, we obtain

$$\operatorname{Re}(\phi_1, \gamma \phi_2) = \operatorname{Re}(\omega_1, \gamma \omega_2) .$$

Here γ may take the values 1 and i , hence

$$(\phi_1, \phi_2) = (\omega_1, \omega_2) \quad (15)$$

for all unit vectors $\phi_1, \phi_2 \in \mathcal{H}$.

We define Ω to be that operator which maps ϕ into ω , i.e., $\Omega \phi = \omega$. Clearly, if the range of Ω is closed, then Equation (15) implies that Ω is an isometry. But the range of Ω is closed by the following argument. In Equation (14) put $\gamma = -1$, $\phi_1 = \phi_m$, $\phi_2 = \phi_n$, $\omega_1 = \omega_m$, and $\omega_2 = \omega_n$, then $\|\phi_m - \phi_n\| = \|\omega_m - \omega_n\|$.

Therefore, if $\Omega \phi_n = \omega_n$ converges to ω , then $\{\phi_n\}$ is Cauchy and there exists a $\phi \in \mathcal{H}$ such that $\Omega \phi = \omega$.

If

$$A_n \equiv \sum_{k=1}^n \lambda_k(\psi_k, \cdot) \phi_k ,$$

then by Equation (12) and property (ii)

$$\mu(A_n) = \sum_{k=1}^n \lambda_k(\Omega \psi_k, \cdot) \Omega \phi_k = \Omega A_n \Omega^* .$$

In general, $A \in \mathcal{B}_1(\mathcal{H})$ is of the form (9). Thus, given $\varepsilon > 0$, choose N such that $\|A_n - A\|_1 < \varepsilon/2$ for all $n \geq N$. Then

$$\begin{aligned} \|\mu(A) - \Omega A \Omega^*\|_1 &\leq \|\mu(A) - \mu(A_n)\|_1 + \|\Omega A_n \Omega^* - \Omega A \Omega^*\|_1 \\ &= 2 \|A_n - A\|_1 < \varepsilon . \end{aligned}$$

It follows that

$$\mu(A) = \Omega A \Omega^* = \sum_{k=1}^{\infty} \lambda_k(\Omega \psi_k, \cdot) \Omega \phi_k \quad (16)$$

for all $A \in \mathcal{B}_1(\mathcal{H})$.

Clearly,

$$\Omega \Omega^* \mu(A) = \mu(A) = \mu(A) \Omega \Omega^* ,$$

so $F = \Omega \Omega^*$ reduces $\mu(A)$. Suppose there exists a projection $E < F$ which also reduces all $\mu(A)$. Choose ω_1 in the range of E and ω_2 in the range of $F - E$. Then for the operator $\mu(A_{12}) = (\omega_2, \cdot) \omega_1$ we have

$$0 = \mu(A_{12}) E = E \mu(A_{12}) = \mu(A_{12}) \neq 0 .$$

Therefore, $F = \Omega \Omega^*$ is the smallest projection which reduces all the operators $\mu(A)$. This proves Theorem 3.

Theorem 4 The asymptotic condition (A) is satisfied if and only if, given a vector ϕ , there exists a vector ψ ($\psi = \Omega \phi$) and a complex function ξ_t of modulus 1 such that

$$\|\xi_t X_t \phi - \psi\| \rightarrow 0$$

as $t \rightarrow \mp \infty$.

Proof

Suppose $\xi(t) X_t \phi \rightarrow \psi$ strongly. Using Lemma 1 and the fact that $X_t P_\phi X_t^*$ and P_ψ are projections with one-dimensional range, we observe

$$\|X_t P_\phi X_t^* - P_\psi\|_1 = 2(1 - |(X_t \phi, \psi)|^2)^{1/2}, \quad (17)$$

since

$$\begin{aligned} \|P_\psi X_t P_\phi X_t^* P_\psi\|_1 &= \text{Tr } P_\psi X_t P_\phi X_t^* = (\psi, P_\psi X_t P_\phi X_t^* \psi) = (X_t^* \psi, P_\phi X_t^* \psi) \\ &= (X_t^* \psi, (\phi, X_t^* \psi) \phi) = |(X_t \phi, \psi)|^2. \end{aligned}$$

Now $\xi(t) X_t \phi \rightarrow \psi$ strongly implies $|(\xi(t) X_t \phi, \psi)| = |(X_t \phi, \psi)| \rightarrow \|\psi\|^2 = 1$.

Therefore, $\|X_t P_\phi X_t^* - P_\psi\|_1 \rightarrow 0$ by Equation (17).

In general, any $W \in \mathcal{W}(\mathcal{H})$ is of the form

$$\sum_{k=1}^{\infty} \lambda_k P_{\{\phi_k\}}$$

where ϕ_1, ϕ_2, \dots are a sequence of orthonormal states with respective probabilities $\lambda_1, \lambda_2, \dots, \lambda_k > 0$ for all k , and

$$\sum_{k=1}^{\infty} \lambda_k = 1.$$

If we take

$$W' = \sum_{k=1}^{\infty} \lambda_k P_{\psi_k}$$

where $\psi_k = s - \lim \xi(t) X_t \phi_k$, then

$$\begin{aligned} \|X_t W X_t^* - W'\|_1 &= \left\| \sum_{k=1}^{\infty} \lambda_k (X_t P_{\phi_k} X_t^* - P_{\psi_k}) \right\|_1 \\ &\leq \sum_{k=1}^N \lambda_k \|X_t P_{\phi_k} X_t^* - P_{\psi_k}\|_1 + \sum_{k=N+1}^{\infty} \lambda_k \|X_t P_{\phi_k} X_t^* - P_{\psi_k}\|_1 \end{aligned}$$

Given $\varepsilon > 0$, we choose N sufficiently large so that

$$\sum_{k=N+1}^{\infty} \lambda_k < \varepsilon/4,$$

then choose T sufficiently large so that $\|X_t P_{\phi_k} X_t^* - P_{\psi_k}\|_1 < \varepsilon/2$ for all $|t| \geq T$ and for all $k = 1, 2, \dots, N$. Then

$$\|X_t W X_t^* - W'\|_1 < \varepsilon/2 \sum_{k=1}^N \lambda_k + 2 \sum_{k=N+1}^{\infty} \lambda_k < \varepsilon.$$

It follows that the asymptotic condition (A) is satisfied.

Using Theorem 3 with the asymptotic condition (A) and Equation (8), we obtain

$$\|X_t A X_t^* - \Omega A \Omega^*\|_1 \rightarrow 0 \quad (18)$$

for all $A \in \mathcal{B}_1(\mathcal{H})$. In particular, for all rays $P = P_\phi$

$$\|X_t P X_t^* - \Omega P \Omega^*\|_1 \rightarrow 0. \quad (19)$$

If we define $Y_t \equiv X_t^* \Omega$, then the continuous one-parameter family of isometric operators Y_t satisfy

$$\|PY_t - Y_t P\|_1 \rightarrow 0. \quad (20)$$

But by Lemma 1 (compare Equation (17))

$$\|PY_t - Y_t P\|_1 = 2(1 - |(\phi, Y_t \phi)|^2)^{1/2},$$

so that

$$|(\phi, Y_t \phi)| = \left[1 - \frac{1}{4} \|PY_t - Y_t P\|_1^2\right]^{1/2} \rightarrow 1 \text{ as } t \rightarrow \mp \infty.$$

If we choose

$$\xi_t(\phi) = \frac{(\phi, Y_t \phi)}{|(\phi, Y_t \phi)|},$$

then $|\xi_t(\phi)| = 1$, and

$$(\phi, \xi_t^*(\phi) Y_t \phi) = |(\phi, Y_t \phi)| \rightarrow 1$$

as $t \rightarrow \mp \infty$, and for all $\phi \in \mathcal{H}$. But then

$$\|\xi_t^*(\phi) Y_t \phi - \phi\|^2 = 2 - 2 \operatorname{Re}(\phi, \xi_t^*(\phi) Y_t \phi) \rightarrow 0,$$

i.e.,

$$\|Y_t \phi - \xi_t(\phi) \phi\| \rightarrow 0 \text{ as } t \rightarrow \mp \infty. \quad (21)$$

We now show that $\xi_t = \xi_t(\phi)$ is independent of ϕ . For a *fixed* cyclic vector $\phi_0 \neq 0$ the set $\{A \phi_0 \mid A \in \mathcal{B}_1(\mathcal{H})\}$, is a dense linear manifold \mathcal{M} in \mathcal{H} , i.e., $\overline{\{A \phi_0\}} = \mathcal{H}$, $A \in \mathcal{B}_1(\mathcal{H})$. Given any vector $\phi \in \mathcal{M}$, we choose $A \in \mathcal{B}_1(\mathcal{H})$ such that $\phi = A \phi_0$. Then since $\xi_t(\phi_0) \phi = \xi_t(\phi_0) A \phi_0 = A \xi_t(\phi_0) \phi_0$,

$$\begin{aligned} \|Y_t \phi - \xi_t(\phi_0) \phi\| &\leq \|Y_t A \phi_0 - A Y_t \phi_0\| + \|A Y_t \phi_0 - A \xi_t(\phi_0) \phi_0\| \\ &\leq \|Y_t A - A Y_t\| \cdot \|\phi_0\| + \|A\| \cdot \|Y_t \phi_0 - \xi_t(\phi_0) \phi_0\| \\ &\leq \|Y_t A - A Y_t\|_1 \cdot \|\phi_0\| + \|A\|_1 \cdot \|Y_t \phi_0 - \xi_t(\phi_0) \phi_0\|. \end{aligned}$$

Letting $t \rightarrow \mp \infty$, the first term on the right goes to zero by Equation (18) and the second term goes to zero by Equation (21). Therefore,

$$\|Y_t \phi - \xi_t(\phi_0) \phi\| \rightarrow 0 \text{ for all } \phi \in \mathcal{M}. \quad (22)$$

For any given $\phi \in \mathcal{H}$ choose $\{\phi_n\}$ such that $\phi_n \rightarrow \phi$, $\phi_n \in \mathcal{M}$. Then

$$\begin{aligned} \|Y_t \phi - \xi_t(\phi_0) \phi\| &\leq \|Y_t \phi - Y_t \phi_n\| + \|Y_t \phi_n - \xi_t(\phi_0) \phi_n\| + \|\xi_t(\phi_0) \phi_n - \xi_t(\phi_0) \phi\| \\ &\leq 2 \|\phi - \phi_n\| + \|Y_t \phi_n - \xi_t(\phi_0) \phi_n\| \rightarrow 0. \end{aligned}$$

Consequently, $\xi_t = \xi_t(\phi_0)$ is independent of ϕ and

$$\|\xi_t X_t \phi - \Omega \phi\| = \|Y_t \phi - \xi_t \phi\| \rightarrow 0$$

for all $\phi \in \mathcal{H}$, q.e.d.

Corollary The asymptotic condition (A) implies

(i) for some real constant α

$$\lim_{t \rightarrow \mp \infty} \frac{\xi_{t+\tau}}{\xi_t} = e^{i\alpha\tau} \text{ for all } \tau.$$

(ii) the intertwining property holds in the sense

$$e^{i\alpha t} \Omega U_t = V_t \Omega.$$

(iii) ξ_t is a differentiable function of t .

Proof By Theorem 4 we know

$$\lim_{t \rightarrow \mp \infty} \|\xi_t X_t \phi - \Omega \phi\| = 0 \quad (23)$$

and

$$\lim_{t \rightarrow \mp \infty} \|\xi_{t+\tau} X_{t+\tau} \phi - \Omega \phi\| = 0 \text{ for all } \tau. \quad (24)$$

By the group property of U_t and V_t we have

$$X_{t+\tau} = V_{t+\tau}^* U_{t+\tau} = V_\tau^* V_t^* U_t U_\tau = V_\tau^* X_t U_\tau.$$

Then

$$\begin{aligned} \|\bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi - V_\tau \Omega \phi\| &\leq \|\bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi - \xi_{t+\tau} X_t U_\tau \phi\| \\ &\quad + \|\xi_{t+\tau} X_t U_\tau \phi - V_\tau \Omega \phi\| \\ &= \|\Omega \psi - \xi_t X_t \psi\| + \|\xi_{t+\tau} X_{t+\tau} \phi - \Omega \phi\| \end{aligned}$$

where $\psi = U_\tau \phi$ in the first term on the right.

Letting $t \rightarrow \mp \infty$ and using (23) and (24) we obtain

$$\lim_{t \rightarrow \mp \infty} \|\bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi - V_\tau \Omega \phi\| = 0. \quad (25)$$

Therefore, given $\varepsilon > 0$, there exists a $T > 0$ such that $|t|, |t'| \geq T$ implies

$$\begin{aligned} |\bar{\xi}_t \xi_{t+\tau} - \bar{\xi}_{t'} \xi_{t'+\tau}| &= |\bar{\xi}_t \xi_{t+\tau} - \bar{\xi}_{t'} \xi_{t'+\tau}| \cdot \|\Omega U_\tau \phi\| \\ &= \|\bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi - \bar{\xi}_{t'} \xi_{t'+\tau} \Omega U_\tau \phi\| \\ &\leq \|\bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi - V_\tau \Omega \phi\| + \|V_\tau \Omega \phi - \bar{\xi}_{t'} \xi_{t'+\tau} \Omega U_\tau \phi\| < \varepsilon, \end{aligned}$$

i.e., $(\bar{\xi}_t \xi_{t+\tau})$ is Cauchy convergent. Thus

$$\lim_{t \rightarrow \mp \infty} \frac{\xi_{t+\tau}}{\xi_t} = \lim_{t \rightarrow \mp \infty} \bar{\xi}_t \xi_{t+\tau} \equiv \omega(\tau) \quad (26)$$

exists, and

$$\begin{aligned} \|\omega(\tau) \Omega U_\tau \phi - V_\tau \Omega \phi\| &\leq \|\omega(\tau) \Omega U_\tau \phi - \bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi\| \\ &\quad + \|\bar{\xi}_t \xi_{t+\tau} \Omega U_\tau \phi - V_\tau \Omega \phi\| \rightarrow 0 \end{aligned}$$

as $t \rightarrow \mp \infty$. Since the left side of this equation is independent of t , we have

$$\omega(\tau) \Omega U_\tau \phi = V_\tau \Omega \phi \text{ for all } \phi \in \mathcal{H} \text{ and all } \tau. \quad (27)$$

It follows from Equation (27) that $\omega(\tau) \phi = U_\tau^* \Omega^* V_\tau \Omega \phi$ is continuous in τ since U_τ and V_τ are strongly continuous in τ . Also,

$$\omega(\tau_1 + \tau_2) = \lim_{t \rightarrow \mp \infty} \frac{\xi(t + \tau_1 + \tau_2)}{\xi(t)} = \lim_{t \rightarrow \mp \infty} \frac{\xi(t + \tau_1 + \tau_2)}{\xi(t + \tau_2)} \frac{\xi(t + \tau_2)}{\xi(t)} = \omega(\tau_1) \omega(\tau_2).$$

Consequently, $\omega(\tau) = e^{i\alpha\tau}$ for some real constant α . With this substitution, Equations (26) and (27) become respectively (i) and (ii).

By the definition of ξ_t we have

$$\xi_t = \xi_t(\phi_0) = \frac{(\phi_0, Y_t \phi_0)}{|(\phi_0, Y_t \phi_0)|} = \frac{(X_t \phi_0, \Omega \phi_0)}{|(X_t \phi_0, \Omega \phi_0)|}.$$

Since $X_t \phi_0 = V_t^* U_t \phi_0$ is differentiable for $\phi_0 \in \mathcal{D}(U_t)$.

$(X_t' \phi_0 = i V_t^* (H - H_0) U_t \phi_0)$, it is clear that ξ_t is a differentiable function of t , q.e.d.

Theorem 4 shows that the new asymptotic condition is equivalent to the old asymptotic condition (cf. [2]) with the addition of a phase factor ξ_t . Also, it is clear that H_0 and $H = H_0 + cI$ will satisfy the new asymptotic condition because, in this case, $\xi_t = e^{ict}$. We point out that this is not the only possible choice of phase factor. For example, $\xi_t = \exp(ic \cdot \log t)$, c a real constant, is allowable.

Finally, we remark that the isometries Ω_\pm obtained by Theorem 3 for the two limits $t \rightarrow \mp \infty$ are a slightly more general definition of the so-called *wave operators* introduced into scattering theory by Møller. Also, the scattering operator may be defined by $S = \Omega_-^* \Omega_+$ as was done in [2].

6. Acknowledgments

This paper was written during a visit of the authors at the Battelle Memorial Institute in Seattle, Washington. We are very grateful to Battelle for financial support which made this visit possible.

We have greatly benefited from correspondence with Professor A. LENARD of the University of Indiana on various aspects of this problem. The 'only if' part of Theorem 4 was first proved by him using a different method, and the Corollary of Theorem 4 is entirely due to him. The proof of Theorem 3 is based on ideas due to CLASINE VAN WINTER and Professor J. A. STAMPFLI.

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