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ABSTRACT

A great deal of interest has been shown recently in the problem of incorporating bound states in relativistic field theories. It is the purpose of this article to point out that if one second-quantizes nonrelativistic quantum mechanics, it becomes amenable to treatments similar to those proposed for relativistic theories. Since nonrelativistic quantum mechanics is much better understood than the relativistic theories, it is possible to test any suggestions made for discussing the latter problem by applying them to the simpler model. In the course of such an investigation it is found that a method proposed by Zimmerman for finding the commutation relations for the in and out operators contains an error. The investigation also suggests that none of the methods so far proposed for introducing in-out operators for bound states seems entirely satisfactory. It is suggested that the procedure used for the nonrelativistic problem has a natural generalization to the relativistic case, and this is outlined.

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I. INTRODUCTION

We wish to discuss nonrelativistic quantum mechanics with two-body interactions using the in-out operator formalism.¹ These techniques are now being used a great deal for relativistic field theories.^{2, 3} In particular, we shall address ourselves to the problem of introducing such operators for bound states both because of the intrinsic interest of such a development and because an example which can be treated rigorously should help in the evaluation of suggestions for treating the relativistic problem.

In any quantum-mechanical problem it is necessary to exercise some care in defining the appropriate Hilbert space. If the Hilbert space is not restricted in some way, it is impossible to obtain an eigenvalue problem. It is convenient, and appropriate, in nonrelativistic quantum mechanics to admit to the Hilbert space only normalizable state vectors. With such a restriction on the Hilbert space, it is possible to justify certain manipulations of the original operator equations of motion and commutation relations. Typically it becomes possible to justify the neglect of certain surface terms, or to assure the validity of changing the order of certain limiting processes, or to guarantee the existence of certain expressions. The operator identities which are obtained with the aid of such manipulations are said to

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be valid in the sense of weak convergence. That is, they lead to correct expressions for matrix elements taken between normalizable state vectors. All the equations in this paper are valid at least in this sense. Many of the operator equations are true for a less restricted Hilbert space. We shall make no systematic attempt to examine the extent to which the normalizability condition on the Hilbert space may be relaxed for the various equations.

This paper is divided into six sections. In Section II the second quantized form of nonrelativistic quantum mechanics is outlined. Although this procedure should be familiar to everyone,⁴ the authors discovered in conversation that this was frequently not so. Our discussion of this problem is formulated in such a way as to provide a convenient starting point for the subsequent analysis. The third section is devoted to determining the conditions necessary to insure that the field operators in the theory possess asymptotic forms. Appropriate definitions of the in and out operators are then given. In the fourth section it is pointed out that the limiting processes involved in defining the asymptotic operators cannot be uniformly convergent because of the invariance of the theory under time translation. As a result, it is necessary to exercise caution in the order of taking limits. With this in mind, suitable methods, based on a suggestion by Zimmermann, for finding the commutation relations of the in and out operators are found. The fifth section is concerned with the definition and evaluation of the S matrix and the final section is reserved for some concluding remarks. There is an appendix in which the properties of nonrelativistic wave packets are discussed.

II. NONRELATIVISTIC QUANTUM MECHANICS

The second-quantized form of nonrelativistic quantum mechanics is described in terms of the field operator $\psi(\underline{x}t)$ and its Hermitian conjugate $\psi^*(\underline{x}t)$. These operators satisfy the equations of motion

$$\frac{i\partial}{\partial t} \psi(\underline{x}, t) + \frac{\partial^2}{\partial \underline{x}^2} \psi(\underline{x}, t) - \int d\underline{y} \psi^*(\underline{y}t) V(\underline{x}-\underline{y}) \psi(\underline{y}t) \psi(\underline{x}, t) = 0, \quad (1).$$

and the equation obtained from the above by Hermitian conjugation. These operator equations are defined relative to a Hilbert space for which the various operations indicated may be defined.⁵ For a large class of potentials, this restriction is not severe. However, for singular potentials (for example an infinite repulsive core) it is necessary to restrict the Hilbert space in an appropriate manner. In what follows we shall assume that such restrictions on the Hilbert space are imposed when necessary.

In addition to the equations of motion, it is necessary to specify the equal-time commutation, or anticommutation, relations. Since the case of Bose statistics permits a more concise treatment, we shall consider the commutation relations

$$[\psi(\underline{x}, t), \psi^*(\underline{x}'t)] = \delta(\underline{x}-\underline{x}') \quad (2)$$

and

$$[\psi(\underline{x}, t) \psi(\underline{x}', t)] = [\psi^*(\underline{x}t) \psi^*(\underline{x}'t)] = 0 \quad (3)$$

Since the results obtained for Fermi statistics are quite interesting, we shall simply quote the results for Fermi statistics.

The Hilbert space appropriate to the problem is most readily introduced in terms of the positive definite number operator,⁶

$$N(t) = \int d\underline{x} \psi^*(\underline{x}, t) \psi(\underline{x}, t). \quad (4)$$

The following commutation relations are easily proven:

$$[N(t), \psi(\underline{x}, t)] = -\psi(\underline{x}, t) \quad (5)$$

and

$$[N(t), \psi^*(\underline{x}, t)] = \psi^*(\underline{x}, t). \quad (6)$$

From the positive definiteness of $N(t)$ and these commutation relations, the existence of a vacuum state with the following properties is easily inferred:

$$N(t) | \text{vac} \rangle = 0, \quad (7)$$

and

$$\psi(\underline{x}, t) | \text{vac} \rangle = 0. \quad (8)$$

The requirement that the vacuum state thus found be unique and time-independent, so that Eq. (8) holds for all times, is sufficient to define the Hilbert space. We consider then the set of normalizable state vectors formed by applying the operators $\psi^*(\underline{x}, t)$ and $\psi(\underline{x}, t)$ to the vacuum. Thus, a typical state vector would be

$$\int d\underline{x} d\underline{x}' d\underline{x}'' G(\underline{x}, \underline{x}', \underline{x}'', t, t', t'') \psi^*(\underline{x}, t) \psi^*(\underline{x}', t') \psi^*(\underline{x}'', t'') | \text{vac} \rangle, \quad (9)$$

where the function G is suitably restricted.

In the usual approach to nonrelativistic quantum mechanics one does not generally consider state vectors which are formed by the application to the vacuum of creation operators for different times. We shall find that the simplest procedure is to consider first only the case in which all the times are equal and then express states such as given in Eq. (9) in terms of the equal-time states.

Consider the set of operators

$$\psi_a^*(t) = \int d\underline{x} f_a(\underline{x}, t) \psi^*(\underline{x}, t), \quad (10)$$

where the set of functions $f_a(\underline{x}, t)$ forms a complete and normalizable set

of wave packets having the properties

$$\int d\underline{x} f_a^*(\underline{x}t) f_\beta(\underline{x}, t) = \delta_{a\beta} \quad (11)$$

and

$$\sum_a f_a(\underline{x}, t) f_a^*(\underline{x}'t) = \delta(\underline{x} - \underline{x}'). \quad (12)$$

The time dependence of $f_a(\underline{x}t)$ is given by the free-field equation

$$i \frac{\partial}{\partial t} f_a(\underline{x}, t) + \frac{\partial^2}{\partial \underline{x}^2} f_a(\underline{x}t) = 0.$$

The construction of such a set of functions and their properties is discussed in an appendix. In what follows we need their asymptotic properties, which are that, for large $|t|$,

$$|f_a(\underline{x}, t)| \sim t^{-3/2} \left| \hat{f}_a\left(\frac{\underline{x}}{2t}\right) \right|, \quad (13)$$

where $\hat{f}$ is the Fourier transform of f and is therefore also a square integrable function of its argument. Also for large $|\underline{x}|$, $f_a(\underline{x}, t)$ goes to zero.

The equation of motion for $\psi_a^*(t)$ is then easily found to be

$$\begin{aligned} -i \frac{\partial}{\partial t} \psi_a^*(t) &= \int d\underline{x} d\underline{y} \psi^*(\underline{x}t) \psi^*(\underline{y}t) V(\underline{x}-\underline{y}) \psi(\underline{y}t) f_a(\underline{x}, t) \\ &\equiv J_a^*(t). \end{aligned} \quad (14)$$

In deriving Eq. (14) we have used the asymptotic properties of $f_a(\underline{x}t)$ and the normalizability of the state vectors in order to justify the neglect of the surface term

$$\int d\underline{x} \left\{ f_a(\underline{x}t) \frac{\partial^2}{\partial \underline{x}^2} \psi^*(\underline{x}t) - \frac{\partial^2 f_a(\underline{x}t)}{\partial \underline{x}^2} \psi^*(\underline{x}t) \right\}. \quad (15)$$

It is possible to write Eq. (14) in the integral form

$$\psi_a^*(t_1) - \psi_a^*(t_2) = i \int_{t_2}^{t_1} dt J_a^*(t). \quad (16)$$

Since $J_a^*(t)$ has a destruction operator at the right,

$$J_a^*(t) |vac\rangle = 0, \quad (17)$$

and therefore the state

$$|a\rangle \equiv \psi_a^*(t) |vac\rangle \quad (18)$$

is time-independent. These states are normalized so that

$$\langle a, \beta \rangle = \delta_{a\beta}. \quad (19)$$

The set of states $|a\rangle$ forms a complete set for all one-particle normalizable states. Consider the state

$$|g(t)\rangle \equiv \int d\underline{x} g(\underline{x}, t) \psi^*(\underline{x}, t) |vac\rangle, \quad (20)$$

with

$$\int d\underline{x} |g(\underline{x}, t)|^2 \quad (21)$$

finite. Then we have

$$g(\underline{x}, t) = \sum_a g_a(t) f_a(\underline{x}, t) \quad (22)$$

where

$$g_a(t) = \int d\underline{x} f_a^*(\underline{x}, t) g(\underline{x}, t). \quad (23)$$

Hence we obtain

$$\begin{aligned} |g(t)\rangle &= \sum_a \int d\underline{x} g_a(t) f_a(\underline{x}, t) \psi^*(\underline{x}, t) |vac\rangle \\ &= \sum_a g_a(t) |a\rangle, \end{aligned} \quad (24)$$

with

$$\sum_a |g_a(t)|^2 = \int d\underline{x} |g(\underline{x}, t)|^2 \quad (25)$$

and finite.

The two-body states can be treated in a similar manner. We consider the Schrödinger equation

$$\left(i \frac{\partial}{\partial t} + \frac{\partial^2}{\partial \underline{x}^2} + \frac{\partial^2}{\partial \underline{y}^2} - V(\underline{x}-\underline{y}) \right) \phi(\underline{x}, \underline{y}, t) = 0, \quad (26)$$

then form the operator

$$\psi_2^*(t) = (2!)^{-1} \int d\underline{x} \int d\underline{y} \phi(\underline{x}, \underline{y}, t) \psi^*(\underline{x}t) \psi^*(\underline{y}t). \quad (27)$$

The equation of motion for $\psi_2^*(t)$ is

$$-i \frac{\partial}{\partial t} \psi_2^*(t) = (2!)^{-1/2} \int d\underline{x} d\underline{y} d\underline{z} \psi^*(\underline{x}t) \psi^*(\underline{y}t) \psi^*(\underline{z}, t) \quad (28)$$

$$[V(\underline{z}-\underline{x}) + V(\underline{x}-\underline{y})] \psi(\underline{z}, t) \phi(\underline{x}, \underline{y}, t) \equiv J_2^*(t).$$

The current $J_2^*(t)$ has a destruction operator on the right as a result of the fact that $\phi(\underline{x}, \underline{y}, t)$ satisfies Eq. (26). The neglect of surface terms which is involved in deriving Eq. (28) can be justified as before. The integral form of Eq. (28) is then

$$\psi_2^*(t_1) - \psi_2^*(t_2) = i \int_{t_2}^{t_1} dt J_2^*(t), \quad (29)$$

and as before, the state

$$|2\rangle = \psi_2^*(t) |vac\rangle \quad (30)$$

is time-independent.

For a certain class of interactions, the solutions of the Schrödinger equation (26) can be divided into two groups corresponding to bound states and to scattering states. The scattering states are conveniently labeled by their behavior at large times,

$$\lim_{t \rightarrow \pm \infty} \phi_{\alpha\beta}^{\text{out}}(\underline{x}\underline{y}, t) = (2!)^{-1/2} (f_{\alpha}(\underline{x}t) f_{\beta}(\underline{y}t) + f_{\alpha}(\underline{y}t) f_{\beta}(\underline{x}t)). \quad (31)$$

The bound-state functions are conveniently written as the product of a function of the center-of-mass coordinate and a function of the internal coordinate

$$\phi_{a2}(\underline{x}, \underline{y}, t) = f_{a2} \left(\frac{\underline{x} + \underline{y}}{2}, t \right) \phi(E_{a2}, \underline{x} - \underline{y}), \quad (32)$$

where the f 's form a complete set of wave packets satisfying the equation

$$\left(i \frac{\partial}{\partial t} + \frac{1}{2} \frac{\partial^2}{\partial \underline{R}^2} - E_{a2} \right) f_{a2}(\underline{R}, t) = 0 \quad (33)$$

and

$$\left[-2 \frac{\partial^2}{\partial \underline{\rho}^2} + V(\underline{\rho}) \right] \phi(E_{a2}, \underline{\rho}) = E_{a2} \phi(E, \underline{\rho}). \quad (34)$$

The set of energies E_{a2} is that set for which Eq. (34) has normalizable solutions with symmetric functions

$$\phi(E_{a2}, \underline{\rho}) = \phi(E_{a2}, -\underline{\rho}). \quad (35)$$

It is well known that the set of bound-state wave functions and either the in or the out functions form a complete set of properly symmetrized functions for the spatial dependence.

It is appropriate then to label the operators defined in Eqs. (27) and (28) and the states defined in Eq. (30) by (for example) the set $a2$ and $a\beta$ in. It is then possible to prove that any normalizable two-particle state vector in the Hilbert space, i. e.,

$$\int d\underline{x} \int d\underline{y} G(\underline{x}, \underline{y}, t, t') \psi^*(\underline{x}, t) \psi^*(\underline{y}, t') | \text{vac} \rangle, \quad (36)$$

can be expressed as a linear combination of the set $a2$ and $a\beta$ in. One need only note that the time of the operator $\psi^*(\underline{y}, t')$ can be changed to the time t by using the completeness relation for the one-particle states, and the proof then proceeds as in the one-particle case.

III. THE IN-OUT OPERATORS

Let us now inquire into the question whether the field operators approach limiting operators for large times. Because of the translational invariance of the theory, it is clear that if such limits exist the approach to the limit cannot be uniform. We shall first look at the one-particle operators $\psi_a^*(t)$.

It is clear by inspecting Eq. (16) that the existence of such limits depends on the time dependence of the matrix elements of the current $J_a^*(t)$. If these matrix elements decrease sufficiently rapidly with time, it is possible to define the operators

$$\psi_{a \text{ in}}^* = \lim_{t \rightarrow -\infty} \psi_a^*(t) = \psi_a^*(t) - i \int_{-\infty}^t dt' J_a^*(t') \quad (37)$$

and

$$\psi_{a \text{ out}}^* = \lim_{t \rightarrow +\infty} \psi_a^*(t) = \psi_a^*(t) + i \int_t^{\infty} dt' J_a^*(t'). \quad (38)$$

The matrix elements of the current operator can be estimated as follows. For convenience we repeat the definition of the current, which is

$$J_a^*(t) = \int d\underline{x} \int d\underline{y} \psi^*(\underline{x}t) \psi^*(\underline{y}t) V(\underline{x}-\underline{y}) \psi(\underline{y}t) f_a(\underline{x}t). \quad (39)$$

The matrix element of $J_a^*(t)$ for which ψ destroys a particle in the state a' and the ψ^* 's destroy two particles, which at large times in the past were in the free states β and β' , behaves for large negative times like

$$\int d\underline{x} \int d\underline{y} f_{\beta}^*(\underline{x}t) f_{\beta'}^*(\underline{y}t) V(\underline{x}-\underline{y}) f_{a'}(\underline{y}t) f_a(\underline{x}t).$$

The time dependence of this matrix element depends on the potential, and we consider a delta-function potential to get an estimate for short-ranged potentials.⁷

In this case, the matrix element behaves like

$$\int d\underline{x} \left| f_a(\underline{x}t) \right|^4.$$

Using the estimate given by Eq. (13) and changing the variable from $\underline{x}$ to $\underline{k} = \frac{\underline{x}}{2t}$, we find

$$\langle J \rangle \sim t^{-3} \int d\underline{k} \left| \hat{f}_a(\underline{k}) \right|^4. \quad (40)$$

For such a time behavior, the integration in Eq. (37) is permissible and the in operator may be defined.

The behavior of the matrix element when the potential has a long-ranged tail may be estimated by considering $V(\underline{x}-\underline{y}) = |\underline{x}-\underline{y}|^{-n}$. Considering the same case as before and using the same procedure, we find

$$\langle J \rangle \sim t^{-n} \int d\underline{k} \int d\underline{\ell} \left| \hat{f}(\underline{k}) \right|^2 \left| \hat{f}(\underline{\ell}) \right|^2 \left| \underline{k}-\underline{\ell} \right|^{-n}. \quad (41)$$

It is clear from this that the in-out operators cannot be defined for Coulomb potentials or for potentials which fall off for large separations more slowly than the Coulomb potential. For the Coulomb potential the time integral in Eq. (37) would be logarithmically divergent.

We may also consider the situation in which the two operators $\psi^* \psi$ annihilate a bound pair of particles in the final state. In this case the time dependence of the matrix element is independent of the potential and is given by

$$\langle J \rangle \sim t^{-3/2} \int d\rho \phi(\rho) V(\rho) \int d\underline{k} \left| \hat{f}_{a2}^* \left(\frac{\underline{k}}{2} \right) \hat{f}_a(\underline{k}) \hat{f}_\beta(\underline{k}) \right|. \quad (42)$$

For such matrix elements it is always permissible to extend the range of integration to $\pm\infty$.

In summary, we have demonstrated that it is permissible to introduce the one-particle in-out operators for potentials which decrease

sufficiently more rapidly than the Coulomb potential for large separation. The same conclusion is reached for the two-particle operators, and the argument can obviously be extended to operators creating a large number of particles.

The properties of the one- and two-particle states which we have established may be summarized as follows. These states are time-independent.

$$|a\rangle = \psi_a^*(t) |vac\rangle = \psi_{a\text{ in}}^* |vac\rangle = \psi_{a\text{ out}}^* |vac\rangle, \quad (43)$$

$$|a2\rangle = \psi_{a2}^*(t) |vac\rangle = \psi_{a2\text{ in}}^* |vac\rangle = \psi_{a2\text{ out}}^* |vac\rangle \quad (44)$$

and

$$|a\beta\text{ in}\rangle = \psi_{a\beta\text{ in}}^*(t) |vac\rangle, \quad (45)$$

$$|a\beta\text{ out}\rangle = \psi_{a\beta\text{ out}}^*(t) |vac\rangle, \quad (46)$$

but

$$|a\beta\text{ in}\rangle \neq |a\beta\text{ out}\rangle. \quad (47)$$

Since the operators $\psi_{a\text{ in}}^*$ are obviously time-independent, it is clear that $\psi_{a\text{ in}}^* \psi_{\beta\text{ in}}^* |vac\rangle$ is independent of time. If we express the operators $\psi_{a\text{ in}}^*$ in terms of the operators $\psi_a^*(t)$ and note that $\psi_{\beta}^*(t) |vac\rangle = \psi_{\beta}^*(t') |vac\rangle$, we find

$$\begin{aligned} \psi_{a\text{ in}}^* \psi_{\beta\text{ in}}^* |vac\rangle &= \{ \psi_a^*(t) \psi_{\beta}^*(t) - \\ &- i \int_{-\infty}^t dt' \int d\underline{x}' d\underline{y}' \psi_{\beta}^*(\underline{x}'t') \psi_a^*(\underline{y}'t') V(\underline{x}'\underline{y}') f_a(\underline{x}'t') f_{\beta}(\underline{y}'t') \} |vac\rangle \end{aligned} \quad (48)$$

It is easy to show directly that the right-hand side of Eq. (48) is time-independent. We may also determine the wave function

$$\phi_{a\beta\text{ in}}(\underline{x}, \underline{y}, t) = (2!)^{-1/2} \langle vac, \psi(\underline{x}t) \psi(\underline{y}t), a\beta\text{ in} \rangle \quad (49)$$

for the state. We find

$$(2!)^{1/2} \phi_{\alpha\beta \text{ in}}(\underline{x}\underline{y}t) = f_{\alpha}(\underline{y}t) f_{\beta}(\underline{x}t) + f_{\alpha}(\underline{x}, t) f_{\beta}(\underline{y}t) \\ - i \int_{-\infty}^t dt' \int d\underline{x}'\underline{y}' G(\underline{x}, \underline{y}, \underline{x}', \underline{y}', t-t') V(\underline{x}'-\underline{y}') f_{\alpha}(\underline{y}'t') f_{\beta}(\underline{x}'t'), \quad (50)$$

where

$$G(\underline{x}, \underline{y}, \underline{x}'\underline{y}', t-t') = \langle \text{vac}, \psi(\underline{x}t) \psi(\underline{y}t) \psi^*(\underline{x}'t') \psi^*(\underline{y}'t'), \text{vac} \rangle. \quad (51)$$

G satisfies the equation

$$\left[i \frac{\partial}{\partial t} + \frac{\partial^2}{\partial \underline{x}^2} + \frac{\partial^2}{\partial \underline{y}^2} - V(\underline{x}-\underline{y}) \right] G(\underline{x}, \underline{y}, \underline{x}', \underline{y}', t-t') = 0 \quad (52)$$

and the boundary condition

$$G(\underline{x}, \underline{y}, \underline{x}', \underline{y}', 0) = \delta(\underline{y}-\underline{x}') \delta(\underline{x}-\underline{y}') + \delta(\underline{y}-\underline{y}') \delta(\underline{x}-\underline{x}'). \quad (53)$$

These equations are sufficient to determine G and to permit the identification of $\phi_{\alpha\beta \text{ in}}$ with the usual time-dependent wave function satisfying boundary conditions at $t \rightarrow -\infty$. It is therefore the same function as occurs in Eq. (31).

Because of the completeness relation for the two-particle states, this is sufficient to establish the identity

$$\psi_{\alpha\beta \text{ in}}^*(t) | \text{vac} \rangle = \psi_{\alpha \text{ in}}^* \psi_{\beta \text{ in}}^* | \text{vac} \rangle \quad (54)$$

The relationship

$$\lim_{t \rightarrow -\infty} \psi_{\alpha\beta \text{ in}}^*(t) = \psi_{\alpha \text{ in}}^* \psi_{\beta \text{ in}}^* \quad (55)$$

is also easily proven.

IV. COMMUTATION RELATIONS OF THE IN-OUT OPERATORS

In attempting to determine the commutation relations of the in and out operators it is necessary to exercise extreme care in taking limits. Because $\psi_a(t)$ does not converge uniformly to $\psi_{a \text{ in}}$ for $t \rightarrow -\infty$, the order of limiting processes is important. When the product of two operators is considered, there is a concealed infinite process which is the sum over intermediate states. As a result, it is possible to have two operators each approach zero and yet have their product remain finite. The simplest example of this is the commutator $[\psi(\underline{x}t), \psi^*(\underline{x}'t)]$, which is independent of time even though the matrix elements of ψ and ψ^* go to zero as $|t| \rightarrow \infty$. For nonrelativistic theories it is only the ordering $\psi \psi^*$ which causes difficulty. The other ordering (normal product ordering) is simpler because the operators must destroy particles already present in the initial or final states. However, care must be exercised even here since the product of operators $\psi\psi$ can destroy either two free particles or a bound state, and these two cases can give rise to different asymptotic behavior. It should be noted that in making estimates we have always considered the operators in their normal product order.

Consider two operators $A(t)$ and $B(t)$ which possess limits

$A_{\text{out}} = \lim_{t \rightarrow +\infty} A(t)$, and similarly for $B(t)$. Following Zimmermann's suggestion, we consider the integral

$$\int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dt' \frac{\partial}{\partial t'} T(A(t) B(t')) = \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dt' T\left(A(t) \frac{\partial B(t')}{\partial t'}\right) - \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} [A(t), B(t)]$$

$$\begin{aligned}
 &= \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' T \left(\frac{\partial A(t)}{\partial t}, \frac{\partial B(t')}{\partial t'} \right) \\
 &\quad + \int dt \left[A(t), \frac{\partial B(t)}{\partial t} \right] \\
 &\quad - \int dt \frac{\partial}{\partial t} [A(t), B(t)] \\
 &= \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' T \left(\frac{\partial A(t)}{\partial t}, \frac{\partial B(t')}{\partial t'} \right) - \int_{-\infty}^{+\infty} dt \left[\frac{\partial A(t)}{\partial t}, B(t) \right].
 \end{aligned} \tag{56}$$

Changing the order of operations interchanges the roles of A and B; one then finds

$$\begin{aligned}
 &\int_{-\infty}^{+\infty} dt' \frac{\partial}{\partial t'} \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} T \left(A(t) B(t') \right) - \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dt' \frac{\partial}{\partial t'} T \left(A(t) B(t') \right) \\
 &= \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} [A(t), B(t)].
 \end{aligned} \tag{57}$$

Upon evaluating the left-hand side of Eq. (57), one obtains

$$\begin{aligned}
 &A_{\text{out}} (B_{\text{out}} - B_{\text{in}}) - (B_{\text{out}} - B_{\text{in}}) A_{\text{in}} \\
 &- \{ B_{\text{out}} (A_{\text{out}} - A_{\text{in}}) - (A_{\text{out}} - A_{\text{in}}) B_{\text{in}} \}.
 \end{aligned}$$

This simplifies to the difference of the commutators of the out and in fields, so that we have

$$[A_{\text{out}}, B_{\text{out}}] - [A_{\text{in}}, B_{\text{in}}] = \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} [A(t), B(t)]. \quad (58)$$

In a similar way we find

$$\begin{aligned} & \int_{-\infty}^{+\infty} dt' \frac{\partial}{\partial t'} \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} T \left(A(t), B(t') C(t'') \right) - \\ & - \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dt' \frac{\partial}{\partial t'} T \left(A(t) B(t') C(t'') \right) \\ & = \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} T \left([A(t), B(t)] C(t'') \right). \end{aligned} \quad (59)$$

Upon evaluating the left-hand side, one obtains

$$[A_{\text{out}}, B_{\text{out}}] C(t'') - C(t'') [A_{\text{in}}, B_{\text{in}}] = \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} T \left([A(t), B(t)] C(t'') \right). \quad (60)$$

Let us now consider the significance of Eqs. (58) and (60). In evaluation of the left-hand side of these equations, the limits $t, t' \rightarrow \pm\infty$ are taken independently; it is therefore possible to identify the limits with the corresponding in or out operators. On the right-hand side the operators appear at the same time. However, they appear in an equal-time commutator, and this is usually easy to simplify.

When Zimmerman considered equations analagous to Eqs. (57) and (59) he indicated that the right-hand sides of these equations were zero. Operating on this assumption, the present authors were led to the conclusion

that the states $\lim_{t \rightarrow \infty} \psi_{\alpha\beta}^* \text{ in}(t) | \text{vac} \rangle$ and $\psi_{\alpha}^* \text{ in} \psi_{\beta}^* \text{ in} | \text{vac} \rangle$ were orthogonal. Since this could not be reconciled with the fact that these states are identical, a more careful evaluation of the argument given by Zimmerman was found necessary.

The difficulty involved is partially one of interpretation. The second-order time derivative of a time-ordered product involves delta functions and their derivatives. One consistent mathematical interpretation of such functions is in terms of distribution theory.⁸ A distribution is a sequence of good functions. Good functions are functions which go to zero faster than any power and are differentiable to all orders. With such an interpretation it is correct to say that the right-hand sides of Eq. (57) and (59) are zero. However, because of the presence of the good functions, the contributions from the end points also vanish and one is led to the empty relation that zero equals zero. It is clear that one does not wish to use distribution theory.

It might seem that a similar objection could be made to the derivation given here. This is in fact not true, for the delta functions implicit in our derivation were used as a shorthand notation. That is, in the sequence

$$\begin{aligned} A_{\text{out}} B(t'') - B(t') A_{\text{in}} &= \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} T \left(A(t) B(t') \right) = \\ &= \int_{-\infty}^{+\infty} dt T \left(\frac{\partial A(t)}{\partial t} B(t') \right) + [A(t'), B(t')] \end{aligned}$$

the ambiguous middle term correctly joins the well-defined expressions on the left and right. For a completely clean mathematical statement of the

content of Eqs. (57) to (60), one should consider the identities

$$\int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' T \left(\frac{\partial A(t)}{\partial t} \frac{\partial B(t')}{\partial t'} \right) = \int_{-\infty}^{+\infty} dt' \int_{-\infty}^{+\infty} dt T \left(\frac{\partial A(t)}{\partial t} \frac{\partial B(t')}{\partial t'} \right) \quad (61)$$

and

$$\begin{aligned} & \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' T \left(\frac{\partial A(t)}{\partial t} \frac{\partial B(t')}{\partial t'} C(t'') \right) \\ &= \int_{-\infty}^{+\infty} dt' \int_{-\infty}^{+\infty} dt T \left(\frac{\partial A(t)}{\partial t} \frac{\partial B(t')}{\partial t'} C(t'') \right). \end{aligned} \quad (62)$$

The existence of A_{out} , A_{in} , B_{out} , and B_{in} guarantees the correctness of these relationships, and the evaluation of these integrals provides a precise meaning to the equations we use. Nevertheless, we shall use Eqs. (58) and (60) as a convenient mnemonic.⁹ It might also be remarked that Eqs. (57) and (59) are valid for finite regions $t_2 \sim t$, $t' \sim t_1$ and that they then yield results which are trivial.

Let us now apply these equations to specific examples. Consider $A(t) = \psi_a(t)$, $B(t) = \psi_\beta^*(t)$, $C(t) = \psi_a(t)$. Then Eq. (58) yields

$$[\psi_{a \text{ out}}, \psi_{\beta \text{ out}}^*] - [\psi_{a \text{ in}}, \psi_{\beta \text{ in}}^*] = \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} \delta_{a\beta} = 0. \quad (63)$$

Using this result to simplify the left-hand side of Eq. (60), we obtain

$$[\psi_{a \text{ out}}, \psi_{\beta \text{ out}}^*, \psi_Y(t'')] = \int dt \frac{\partial}{\partial t} T \left(\delta_{a\beta} \psi_Y(t'') \right) = 0. \quad (64)$$

Similarly, by letting $C(t) = \psi_Y^*(t)$, we obtain

$$\left[[\psi_{\alpha \text{ out}}, \psi_{\beta \text{ out}}^*], \psi_{\gamma}^*(t'') \right] = 0. \quad (65)$$

Since the operators $\psi_{\gamma}(t)$ and $\psi_{\gamma}^*(t)$ form an irreducible operator ring, Eqs. (64) and (65) imply that $[\psi_{\alpha \text{ out}}, \psi_{\beta \text{ out}}^*]$ is a c-number and hence equal to its vacuum expectation value. We thus obtain

$$[\psi_{\alpha \text{ out}}, \psi_{\beta \text{ out}}^*] = [\psi_{\alpha \text{ in}}, \psi_{\beta \text{ in}}^*] = \delta_{\alpha\beta}. \quad (66)$$

It is easy to demonstrate

$$[\psi_{\alpha \text{ out}}, \psi_{\beta \text{ out}}] = [\psi_{\alpha \text{ in}}^*, \psi_{\beta \text{ in}}^*] = [\psi_{\alpha \text{ in}}, \psi_{\beta \text{ in}}] = [\psi_{\alpha \text{ out}}^*, \psi_{\beta \text{ out}}^*] = 0. \quad (67)$$

That is, the one-particle in and out operators satisfy free-field commutation relations.

Let us now apply the same technique to the two-particle in and out operators. That is, let $A(t) = \psi_{\alpha 2}(t)$, $B(t) = \psi_{\beta 2}^*(t)$ and $C(t)$ be successively $\psi_{\gamma}(t)$ and $\psi_{\gamma}^*(t)$. It is convenient to examine first the equal-time commutator

$$\begin{aligned} & \frac{1}{2} \left[\int d\underline{x} d\underline{y} \phi_{\alpha 2}^*(\underline{x}, \underline{y}, t) \psi(\underline{x}, t) \psi(\underline{y}, t), \int d\underline{z} d\underline{w} \psi^*(\underline{z}, t) \psi^*(\underline{w}, t) \phi_{\beta 2}(\underline{z}, \underline{w}, t) \right] \\ &= \int d\underline{x} d\underline{y} \phi_{\alpha 2}^*(\underline{x}, \underline{y}, t) \phi_{\beta 2}(\underline{x}, \underline{y}, t) \\ &+ 2 \int d\underline{x} d\underline{y} d\underline{z} \psi^*(\underline{x}, t) \psi(\underline{y}, t) \phi_{\alpha 2}^*(\underline{y}, \underline{z}, t) \phi_{\beta 2}(\underline{x}, \underline{z}, t) \\ &= \delta_{\alpha 2, \beta 2} + 2 \int d\underline{x} d\underline{y} d\underline{z} \psi^*(\underline{x}, t) \psi(\underline{y}, t) \phi_{\alpha 2}^*(\underline{y}, \underline{x}, t) \phi_{\beta 2}(\underline{x}, \underline{z}, t), \end{aligned} \quad (68)$$

where we have put the operators in a normal product order. It is now possible to estimate the asymptotic behavior of the second term on the right-hand side of Eq. (68). Because of the exponential drop-off for the

relative coordinate for the bound-state wave function, it is possible to replace $\underline{x}$ by $\underline{z}$, $(\underline{x} + \underline{z})/2$ by $\underline{z}$, etc. in the arguments of the wave-packet terms. We then find that this term behaves asymptotically like

$$\int d\underline{p} \int d\underline{\eta} \int d\underline{z} \phi_{a2}^*(\underline{p}) \phi_{\beta 2}(\underline{\eta}) |f(\underline{z}, t)|^4 \sim t^{-3}, \quad (69)$$

and hence can be neglected in the integral. Proceeding in this way, it is then possible to show

$$[\psi_{a2 \text{ out}}, \psi_{\beta 2 \text{ out}}^*] = \delta_{a2, \beta 2}, \quad (70)$$

and so on.¹⁰ By letting $A(t) = \psi_{a2}(t)$ and $B(t) = \psi_{\beta}^*(t)$, one is led to

$$[\psi_{a2 \text{ in}}, \psi_{\beta \text{ in}}^*] = 0. \quad (71)$$

Similarly, all the commutators of one-particle in operators and two-particle in operators commute. From this we conclude that the states $\psi_{a2 \text{ in}}^* |vac\rangle$ and $\psi_{a \text{ in}}^* \psi_{\beta \text{ in}}^* |vac\rangle$ are orthogonal.¹¹

If we had used Zimmerman's result it would not have been necessary to consider the asymptotic behavior of the commutator, and the operators $\psi_{a2}^*(t)$ and $\psi_{a\beta \text{ in}}^*(t)$ would have been on an equal footing. One would then be forced to the absurd conclusion that the states $\psi_{a\beta \text{ in in}}^* |vac\rangle$ and $\psi_{a \text{ in}}^* \psi_{\beta \text{ in}}^* |vac\rangle$ were orthogonal. To see why such a conclusion cannot be drawn, let us consider $A(t) = \psi_{a\beta \text{ in}}(t)$, $B(t) = \psi_{a'\beta' \text{ in}}^*(t)$. As before, the appropriate commutator $[A(t), B(t)]$ is given by

$$\delta_{aa'} \delta_{\beta\beta'} + \delta_{a\beta'} \delta_{a'\beta} + 2 \int d\underline{x} d\underline{y} d\underline{z} \psi^*(\underline{x}t) \psi(\underline{y}t) \phi_{a'\beta' \text{ in}}^*(\underline{y}, \underline{z}, t) \phi_{a\beta \text{ in}}(\underline{x}, \underline{z}, t);$$

when the asymptotic value of the second term is examined, one obtains terms of the form

$$\int dx f^*(\underline{x}t) f_a(\underline{x}t) \int d\underline{y} f^*_{\beta'}(\underline{y}t) f(\underline{y}t) \int d\underline{z} f^*_{a'}(\underline{z}t) f_{\beta}(z, t).$$

This term behaves like a constant and therefore contributes to the integral.¹²

Hence the commutators in question are not c-numbers, and the commutators

$$[\psi_{a\beta \text{ in, in}}, \psi^*_{a'\beta' \text{ in, in}}] \text{ and } [\psi_{a\beta \text{ in, out}}, \psi^*_{a'\beta' \text{ in, out}}]$$

are not equal. The operator $\psi_{a\beta \text{ in out}}$ is the limit $t \rightarrow +\infty \psi_{a\beta \text{ in}}(t)$. It can be expressed simply in terms of $\psi_{a' \text{ out}}, \psi_{\beta' \text{ out}}$ and the S matrix, which we will now discuss.

V. REDUCTION FORMULAS AND THE S MATRIX

It is now possible to define the S-matrix in the usual way as the inner product of the in and the out states. Thus, a typical S matrix element is given by

$$\langle a'\beta' \text{ out}, \beta a \text{ in} \rangle = S(a'\beta', \beta a). \quad (72)$$

One can calculate such an S-matrix element by techniques similar to those used in relativistic field theories. We consider

$$\begin{aligned} \int_{-\infty}^{+\infty} dt \langle a' \text{ out}, \frac{\partial \psi_{\beta'}(t)}{\partial t} \beta a \text{ in} \rangle &= \langle a', \psi_{\beta' \text{ out}}, \beta a \text{ in} \rangle \\ &- \langle a' \psi_{\beta' \text{ in}}, \beta a \text{ in} \rangle \\ &= S(a'\beta', \beta a) - \delta_{\beta'a} \delta_{a'\beta} - \delta_{\beta'\beta} \delta_{aa'}. \end{aligned} \quad (73)$$

After simplifying the left-hand side and rearranging terms, one gets

$$S(a'\beta', \beta a) = \delta_{a a'} \delta_{\beta \beta'} + \delta_{a \beta'} \delta_{\beta a'} - i \int_{-\infty}^{+\infty} dt \int d\underline{x} d\underline{y} \left\langle a' \left| f_{\beta'}^*(\underline{x}t) \psi^*(\underline{y}t) V(\underline{x}-\underline{y}) \psi(\underline{y}t) \psi(\underline{x}t) \right| \beta a \text{ in} \right\rangle. \quad (74).$$

Expressing this in terms of wave functions, we get the familiar result

$$S(a'\beta', \beta a) = (a'\beta' \text{ in}, \beta a \text{ in}) - i \int_{-\infty}^{+\infty} dt \int d\underline{x} d\underline{y} (2i)^{-1/2} \left(f_{a'}^*(\underline{y}t) f_{\beta'}^*(\underline{x}t) + f_{a'}^*(\underline{x}t) f_{\beta'}^*(\underline{y}t) \right) \phi_{a\beta \text{ in}}(\underline{x}\underline{y}t) V(\underline{x}-\underline{y}). \quad (75)$$

It should be clear also that the techniques developed here can handle the question of rearrangement collisions very naturally. We do not intend, however, to add to the already extensive literature on this subject.¹³

The extension of this method of evaluating S-matrix elements to systems with many particles is straightforward. One can in such cases get a rather rich variety of equivalent expressions for the S-matrix elements by performing the reductions in different ways.

VI. CONCLUSIONS

We have already adequately discussed the question of determining the commutation relations for the various in and out fields. The net effect is that the theory is described by a set of independent free-field operators $\psi_{a \text{ in}}, \psi_{a2 \text{ in}}, \psi_{a3 \text{ in}} \dots$ and their Hermitian conjugates.¹⁴ The theory can also be described in terms of the out operators, and the physics is introduced by trying to find the relationship between the in and out descriptions.

Our introduction of the bound-state in operator differed in some ways from the approach developed by Zimmermann. We will now discuss these differences and why we were obliged to proceed as we have.

Zimmermann introduces an operator analogous to

$$\psi_{a2z}(\underline{p}, t) = \int d\underline{R} f_{a2}^*(\underline{R}, t) \psi\left(\underline{R} + \frac{\underline{p}}{2}, t\right) \psi\left(\underline{R} - \frac{\underline{p}}{2}, t\right), \quad (76)$$

with its associated current

$$i \frac{\partial}{\partial t} \psi_{a2z}(\underline{p}t) = J_{a2z}(\underline{p}t). \quad (77)$$

Consider now the matrix element

$$\langle \beta 2, J_{a2z}^*(\underline{p}, t) \text{ vac} \rangle = (E_{a2} - E_{\beta 2}) \int d\underline{R} f_{a2}(\underline{R}, t) \phi_{\beta 2}^*(\underline{p}) f_{\beta 2}^*(\underline{R}t). \quad (78)$$

This matrix element has an oscillatory time dependence given by the factor $\exp [i(E_{\beta 2} - E_{a2})t]$. In Zimmermann's paper he considered the special case in which there is only one bound state and hence $E_{a2} = E_{\beta 2}$. For this special case the oscillatory part of the current disappears, and one can expect that the remaining matrix elements of the current go to zero sufficiently rapidly at large times to justify the introduction of the in-out operators. His procedure, however, is not readily extended to the case of more than one bound state. It is our opinion that the interpretation of such oscillatory integrals with the aid of an "adiabatic" cutoff procedure is not valid mathematics and is violently out of keeping with the general techniques adopted here. This is particularly true since the energies E_{a2} and $E_{\beta 2}$ are discrete.

If, for the special case of one bound state, we followed Zimmerman's procedure, we would introduce the in operator $\psi_{a2z \text{ in}}(\underline{\rho})$, which is related to our $\psi_{a2 \text{ in}}$ by

$$\psi_{a2z \text{ in}}(\underline{\rho}) = \phi_{a2}(\underline{\rho}) \psi_{a2 \text{ in}}. \quad (79)$$

Zimmermann would then eliminate the dependence on $\underline{\rho}$ by dividing both sides of the equation by $\phi_{a2}(\underline{\rho})$. Since this is a nonlinear operation, it makes subsequent manipulations very difficult. Our procedure has been to multiply both sides by $\phi_{a2}^*(\underline{\rho})$ and integrate over $\underline{\rho}$. This has the advantage that it is a linear operation and that because of the orthogonality of the ϕ 's, the unwanted terms exhibited in Eq. (72) all drop out.

Nishijima¹⁶ follows a somewhat different technique, although he eliminates the internal coordinate dependence by a procedure similar to ours. However, he does not find it necessary to impose any restrictions other than normalizability on his function ϕ^* . Although we have not been able to understand clearly the relation of Nishijima's procedure to ours, we believe he also will have troubles with Eq. (72) when there are several bound states.

The general lesson to be learned from the above remarks seems to be that, except for the special case of only one bound state, it is necessary to have some knowledge of the internal wave function before it is possible to define in-out operators. The properties of the wave functions which have been most useful are their completeness and orthogonality. The completeness relation can be deduced by taking the vacuum expectation value of the operator identity

$$\left[\psi(\underline{x}', t), [\psi(\underline{y}', t), \psi^*(\underline{y}, t) \psi^*(\underline{x}, t)] \right] = \delta(\underline{x} - \underline{x}') \delta(\underline{y} - \underline{y}') + \delta(\underline{x} - \underline{y}') \delta(\underline{x}' - \underline{y}). \quad (80)$$

The orthogonality relations can be obtained by noting that for matrix elements between two-particle states the operator

$$\int d\underline{x} d\underline{y} \psi^*(\underline{x}, t) \psi^*(\underline{y}, t) \psi(\underline{y}, t) \psi(\underline{x}, t) \quad (81)$$

is equivalent to $2!$.

The first expression (Eq. 80) can be taken over directly for relativistic fermions, and the second has its analog because of baryon conservation. The consequences of Eqs. (80) and (81) are much more difficult to ascertain for the relativistic problem, because the baryon number operator has negative as well as positive eigenvalues. For example, in the nonrelativistic case the only term that contributes to Eq. (80) is $\langle \text{vac}, \psi \psi \psi^* \psi^* \text{vac} \rangle$, whereas all orderings contribute for the relativistic problem.

If it is desired to use Eqs. (80) and (81) in a relativistic problem, then one is led to consider equal-time wave functions,

$$\langle \text{vac}, \psi(\underline{x}, t) \psi(\underline{y}, t), a_2 \rangle. \quad (82)$$

Although this seems a highly nonrelativistic procedure, it is not necessarily undesirable. Hall and Wightman¹⁷ have shown that for a relativistic problem, the matrix element

$$\langle \text{vac}, \psi(\underline{x}_1 t_1) \psi(\underline{x}_2 t_2) \psi^*(\underline{x}_3 t_3) \psi^*(\underline{x}_4 t_4) \text{vac} \rangle \quad (83)$$

can be determined if the matrix element with equal times is known. They could prove such results for matrix elements with up to four operators.

In their proof they used only such properties of the theory as restrictions on the permissible spectrum and causality requirements. For the nonrelativistic problem, a similar result is true with any number of operators. In proving this it is necessary to use the equations of motion. It is not unreasonable to hope that a similar result might be true in the relativistic problem. In any case, for the two-baryon problem, Hall and Wightman's theorem guarantees that no information about the system is lost by considering the equal-time wave functions.

APPENDIX

Wave Packets

The wave-packet functions $f_a(\underline{x}, t)$ can be determined in terms of any complete and orthogonal set of functions $f_a(\underline{x}, 0)$. A suitable choice for the $f_a(\underline{x}, 0)$ would be, for example, the solutions of the harmonic-oscillator problem. The functions $f_a(\underline{x}, t)$ are then defined by

$$f_a(\underline{x}, t) = \int d\underline{x}' H(\underline{x} - \underline{x}', t) f_a(\underline{x}', 0), \quad (A1)$$

where

$$H(\underline{x}, t) = (2\pi)^{-3} \int d\underline{k} e^{i\underline{k} \cdot \underline{x} - i k^2 t} \quad (A2)$$

$$= \frac{1}{8} (\pi t)^{-3/2} e^{i \left(\frac{r^2}{4t} - \frac{3\pi}{4} \right)}. \quad (A3)$$

It is easy to see that the orthogonality and completeness conditions imposed on the wave packets are time-independent. The asymptotic behavior of the wave packets is now easily determined. Neglecting constant factors, we obtain

$$f_a(\underline{x}, t) \sim t^{-3/2} e^{i \frac{\underline{x}^2 m}{2t}} \int d\underline{x}' \exp i \underline{x}' \cdot \frac{m \underline{x}}{t} f_a(\underline{x}', 0) \quad (A4)$$

$$\sim t^{-3/2} e^{i \frac{\underline{x}^2 m}{2t}} \hat{f}_a \left(\frac{m}{t} \underline{x} \right) \quad (A5)$$

where $\hat{f}_a$ is the Fourier transform of $f_a(\underline{x}, 0)$. The dependence on the mass is indicated. The asymptotic behavior is easily understood. The probability of finding a particle at the point $\underline{x}, t$ is proportional to the probability that the particle initially had the correct momentum to get to the point $\underline{x}$ from the origin in a time t . Because of the dependence on $\underline{x}/t$, the wave packet

spreads out, and the over-all time dependence compensates for this spreading out in such a way as to permit the conservation of probability. The oscillatory dependence is necessary to insure that the local expectation value of the moment operator asymptotically approaches $\underline{mx}/t$.

Similar expressions for bound-state wave packets can be obtained. It is necessary only to replace the mass m by the total mass of the bound state and to multiply by an oscillatory term $\exp(-i E_{an} t)$. Since in any matrix element the total mass in the initial state must equal the mass in the final state, the strongly oscillating phase depending on x^2/t always cancels; it therefore does not contribute to the reduction of matrix elements at large times.

REFERENCES AND FOOTNOTES

1. Lehmann, Symanzik and Zimmerman, *Nuovo cimento* 1, 205 (1955).
2. R. Haag, *Phys. Rev.* 112, 669 (1958).
3. W. Zimmermann, *Nuovo cimento* 10, 597 (1958).
4. L. I. Schiff, Quantum Mechanics (McGraw-Hill, New York, 1959) pp. 336-348.
5. That is, matrix elements of ψ must be twice differentiable with respect to its spatial coordinates, and the matrix elements of the $\psi^* \psi \psi$ term must be such that the integral exists.
6. We indicate a time dependence for the number operator although in the context of this paper the number operator does not depend on time. However, in a formulation where the state vectors are not normalizable (plane wave states for example) it is possible to base the theory of the S matrix on the time dependence of $N(t)$. This is the usual procedure since $N(t)$ is expressible in terms of the flux operator. In the formulation adopted here, contributions from spatial surface terms are eliminated, but it becomes necessary to consider surface contributions to the time integrations.
7. The estimate thus obtained can easily be seen to be valid for the contribution to the matrix element from a region of space where $\underline{x-y}$ is restricted to a finite volume and the center-of-mass coordinate integration goes over all space.
8. M. J. Lighthill, Fourier Analysis and Generalised Functions (Cambridge University Press, 1958).
9. It is clear that a second consistent mathematical use of the delta function is as a mnemonic.

10. The commutation relations given by Eq. (66) and the statement that the in operators correspond to free-field operators can be put in a more familiar form by introducing the operator $\psi_{in}(\underline{x}, t) = \sum_a f_a(\underline{x}, t) \psi_{a in}$. In a similar manner for bound states it is possible to introduce an operator $\psi_{E in}(\underline{x}, t) = \sum_{an} f_{an}(\underline{x}, t) \psi_{an, in}$ corresponding to a discrete internal energy E. The sum over wave packets corresponds to a sum over those wave packets associated with the energy E through an equation such as Eq. (33). The operators thus introduced satisfy free-field equations and the usual free-field commutation relations.
11. Similar results hold for Fermi statistics. Thus we may consider the set of in operators corresponding to one-particle states and to many-particle bound states. These operators may be divided into two classes corresponding to association with states having an even or odd number of particles. It is then found that the even operators commute with the odd operators. The set of even operators satisfies free-field commutation relations. The set of odd operators satisfies free-field anticommutation relations. That is, the set of operators behaves like a set of independent free-field operators with the even operators corresponding to bosons and the odd operators to fermions. Relations analogous to Eqs. (57) and (59) may be found, but one must consider separately the various possible combinations of even and odd operators.
12. That is, at $t \rightarrow -\infty$ it approaches one constant, and at $t \rightarrow +\infty$ it approaches another constant. There is then a contribution to the integral equal to the difference of these two results. One can carry this process through in detail and show that the result is consistent with $\lim_{t \rightarrow -\infty} \psi_{a\beta in}(t) = \psi_{a in} \psi_{\beta in}$.

13. For an excellent discussion of scattering theory and in particular of this question, see E. Gerjuoy, *Annals of Physics* 5, 58 (1958).
14. Thus the operator $\psi(xt)$ can be expressed as a sum of normal products of in operators and the coefficients are readily determined once all the matrix elements of $\psi(xt)$ are known. Also the constants of the motion are readily expressed in terms of either the in or the out operators. Thus, the Hamiltonian is a sum of free-field Hamiltonians and the number operators is $N = \sum_a \psi_a^* \psi_a \text{ in } \psi_a \text{ in} + \frac{1}{2} \sum_{a2} \psi_{a2}^* \psi_{a2} \text{ in } \psi_{a2} \text{ in} + \dots$
15. Since such a procedure would introduce $\delta(E_{a2} - E_{\beta 2})$ and for discrete energies, this has no happy interpretation.
16. K. Nishijima, *Phys. Rev.* 111, 995 (1958).
17. D. Hall and A. S. Wightman, *Kgl. Danske Videnskab. Selskab, mat-fys Medd.* 31, paper No. 5 (1957).