

Representation of States in a Field Theory with Canonical Variables*

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We investigate the properties of a functional representation of states for a self-coupled scalar field theory. The assumption is made that all states can be generated by applying functionals of the field at a fixed time ($t=0$) to the vacuum state. It is shown that for the class of models considered the Hamiltonian is uniquely determined by the vacuum functional. The calculation of scalar products between states leads to functional integrals. The measure in this integration over function space is also determined by the vacuum state. Two methods for the evaluation of the functional integrals are discussed. The first one reduces the problem in some simple cases to the solution of an eigenvalue problem for a Hilbert-Schmidt kernel plus a finite number of ordinary integrations. The other one gives a perturbation series.

I. INTRODUCTION

WE want to discuss here some aspects of a field theoretical model of the following type: The basic variables are a scalar field $\varphi(x)$ and its conjugate momentum $\pi(x)$. They shall satisfy the ordinary canonical commutation relations.

$$\begin{aligned} [\pi(x), \varphi(y)] &= -i\delta(x-y), \\ [\varphi(x), \varphi(y)] &= [\pi(x), \pi(y)] = 0. \end{aligned} \quad (1)$$

The Hamiltonian shall be of the form

$$H = \frac{1}{2} \int \pi^2 d^3x + H'(\varphi), \quad (2)$$

where H' is a functional of the field φ only. In particular we could write

$$H' = \frac{1}{2} \int (|\nabla\varphi|^2 + m^2\varphi^2) d^3x + gH^I, \quad (3)$$

and call H^I the interaction Hamiltonian.

We will not discuss here the problems associated with the ultraviolet divergencies which are encountered if H^I is an integral over a point function such as

$$H^I = \int \varphi(x)^4 d^3x. \quad (4)$$

But we consider for instance models of the form

$$H^I = \int \cdots \int h(x_1 \cdots x_4) \varphi(x_1) \cdots \varphi(x_4) d^3x_1 \cdots d^3x_4, \quad (4a)$$

where $h(x_1 \cdots x_4)$ is a smooth "smearing function." We will therefore not assume Lorentz invariance but only invariance under the Euclidean group (translations and rotations in 3-space). It is obvious, however, that any qualitative information about the behavior of the solutions of the above models will also help in the discussion

of a local relativistic field theory like (4) which is just a limiting case of (4a). In fact, this provides part of our motivation.

In the standard treatment of our problem one starts with a decomposition of φ and π into "bare-particle creation and destruction operators" $a^\dagger(k)$, $a(k)$ and represents the states as vectors in the associated Fock space. This seems unfortunate for several reasons. In the first place the quantities $a(k)$, $a^\dagger(k)$ are less well suited to the problem than the original φ and π . In fact it seems extremely difficult to gain any qualitative insight into the nature of the solutions in a scheme which classifies according to the number of bare particles. Secondly the Fock-space treatment cannot be applied directly in a model with vacuum polarization. The nature of this difficulty may be stated in the following way: There are infinitely many inequivalent irreducible representations of the system of commutation relations (1).¹ One particular possibility among this infinite multitude is Fock space. Thus the situation is in marked contrast to wave mechanics where one has to deal only with a finite number of canonical variables q_k , p_k . There one has no representation problem since one knows that all irreducible representations of these operators are equivalent.² Now if the theory is free of ultraviolet divergencies this means, roughly speaking, that the relevant volume of momentum space is finite. If in addition we would put the system into a box to make also the volume of ordinary space finite, then only a finite number of oscillators would be significant and the difficulty would disappear. On the other hand, for an infinitely extended system, it is very easy to see³

¹ This fact was first recognized by K. O. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1953). For the case of the anti-commutation relations it is implicitly contained already in the paper by J. Von Neumann, *Comp. Math.* **6**, 1 (1938). For the commutation relations an indication of the phenomenon may also be found in the paper by L. Van Hove, *Physica* **18**, 145 (1952).

² J. von Neumann, *Math. Ann.* **104**, 570 (1931); F. Rellich, *Gött. Nachr.* 107 (1946).

³ R. Haag, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **29**, No. 12 (1955).

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that the representation appropriate to the case $H^I=0$ (free field) cannot be appropriate to a case with interaction unless H^I is of such a special form that it leaves the unperturbed vacuum invariant. In other words, only for a model without vacuum polarization does the customary "bare-particle Fock space" provide a possible representation in which one can start to calculate. It must be emphasized that the argument just quoted from references does not make use of Lorentz invariance but only of the invariance under translations in space and therefore the difficulty is present even in a convergent nonrelativistic theory as soon as one has vacuum polarization terms in the Hamiltonian.

Therefore if one wants to use Fock space in such a model, one is forced to introduce a finite total volume V and discuss the effect of the limit $V \rightarrow \infty$ at the end. This complication is not very serious for some questions but it is troublesome for others. For instance, while we know that the S -matrix elements must turn out to be independent of V in the limit, the wave functions of physical states contain normalization factors which depend exponentially on the volume. A careful analysis of the volume dependence of various quantities has been made recently within the scope of perturbation theory.⁴

If we want to avoid using a finite box and Fock space in the treatment of the problem, we must find a way to single out that particular representation of (1) which is appropriate to the given Hamiltonian (2). Systematic studies of the relations (1) have been made by Garding and Wightman⁵ and by Segal.⁶ Unfortunately the results of reference 5 are not so convenient for our purpose because in that work the occupation number operators in some discrete basis are taken diagonal. It seems more natural in our problem to diagonalize the fields. This corresponds essentially to Segal's approach. A naive version of some of his methods will therefore appear in this paper, but our assumptions are more specific.

Our approach is exploratory and therefore, apart from Appendix I, mathematically naive.⁷ Its main purpose is to present some useful concepts and discuss their relationships.

II. THE VACUUM FUNCTIONAL

We want the model defined by Eqs. (1) and (2) to satisfy the following requirements:

⁴ L. Van Hove, *Physica* **21**, 901 (1955); **22**, 343 (1956). N. Hugenholtz, *Physica* **23**, 481 (1957); W. R. Frazer and L. Van Hove, *Physica* **24**, 151 (1958).

⁵ L. Garding and A. S. Wightman, *Proc. Natl. Acad. Sci. U. S.* **40**, 617 (1956).

⁶ I. E. Segal, *Trans. Am. Math. Soc.* **88**, 12 (1958); *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **31**, No. 12 (1959).

⁷ Parallel to this work, a mathematically rigorous discussion of the representation problem has been taken up by J. Lew, A. S. Wightman and one of us (R. H.). H. Araki has analyzed some examples in which the connection between the Hamiltonian and the type of representation can be worked out explicitly.

(i) *There exists a discrete (i.e., normalizable) ground state of H , called the vacuum state Ψ_0 , which is invariant under the Euclidean group and under time inversion.*

(ii) *Every other state of our system may be generated by applying some functional of the field operators $\varphi(x)$ to the vacuum.*

Thus

$$\Psi = F(\varphi)\Psi_0.$$

In other words, it is assumed that we can create all the states from the vacuum without making use of the momentum operators. A precise mathematical formulation of assumption (ii) will be given in Appendix I. Here we shall be content to illustrate the meaning of this assumption and the consequences by analogy with the quantum mechanics of a single oscillator (i.e., we have only one pair of canonical variables p, q). We take q diagonal and consider the wave function of the ground state $\psi_0(q)$. Since ψ_0 has no nodes, every other state can be approximated arbitrarily well by $F(q)\psi_0(q)$, where the operator F may be chosen as a bounded, continuous function of q . The following two consequences are seen immediately:

(1) If G is any operator which commutes with q then

$$G\psi_0 \neq 0 \quad \text{unless} \quad G=0. \quad (5)$$

(2) There exists a function $L(q)$ such that

$$[p - iL(q)]\psi_0 = 0. \quad (6)$$

In fact, if we write $\psi_0 = e^{-\Lambda(q)}$, then $L = d\Lambda/dq$.

In our field theoretical problem we draw two analogous conclusions from (ii). In particular we assert that there exists a functional of the field, called Λ , such that

$$[\pi(x) - iL(x)]\Psi_0 = 0, \quad (7)$$

with

$$L(x) = \delta\Lambda/\delta\varphi(x). \quad (8)$$

Because of the invariance under time reflection, Λ must be a *real* functional of φ so that Λ and $L(x)$ are Hermitian operators.

What is the connection between Λ and the Hamiltonian H ? Making use of the special form (2) of H and of the commutation relations (1), we can write

$$H = \frac{1}{2} \int [\pi(x) + iL(x)][\pi(x) - iL(x)] d^3x + F(\varphi).$$

If E_0 is the vacuum energy then (7) tells us

$$[F(\varphi) - E_0]\Psi_0 = 0.$$

Since, however, $F(\varphi) - E_0$ commutes with all the $\varphi(x)$ we conclude from (ii) that the operator $F - E_0$ itself must vanish. We will from now on take $E_0 = 0$.⁸ Then

⁸ This is clearly necessary if we want finite results in the case of an infinite volume since E_0 must be proportional to V . It also does not restrict the generality; if the originally given formal Hamiltonian gives $E_0 \neq 0$, one must consider $H - E_0$ as the proper Hamiltonian.

we learn that

$$H = \int A^\dagger(x) A(x) d^3x, \quad (9)$$

with

$$A(x) = 2^{-1/2} [\pi(x) - iL(x)]. \quad (10)$$

If we multiply (9) out and compare with (2) we get the following explicit relation between H' and Λ

$$\int L(x)^2 d^3x - \int \frac{\delta L(x)}{\delta \varphi(x)} d^3x = 2H'. \quad (11)$$

We want to point out one possible use of this equation. If one wants to study the mathematical structure of models of type (1), (2), it may be advantageous to consider Λ rather than H as given. H' can then be calculated directly from (11) while an assumed H' does not, in general, yield a closed expression for Λ . Let us examine finite polynomials for Λ of the form

$$\Lambda = \sum_{n=2}^N \frac{1}{n!} \lambda_n(x_1 \cdots x_n) \varphi(x_1) \cdots \varphi(x_n) d^3x_1 \cdots d^3x_n. \quad (12)$$

The simplest choice, $N=2$, yields a theory of noninteracting particles which have an energy-momentum relation

$$E = \lambda(p)^2, \quad (13)$$

where $\lambda(p)$ is the Fourier transform of $\lambda_2(x_1 - x_2)$. Polynomials of odd degree are ruled out by the requirement (19) below. The simplest nontrivial choice is therefore $N=4$ which gives a polynomial of sixth degree for H . The finite polynomials (12) for Λ have the serious drawback that (except in the trivial case $N=2$) they do not yield theories which are even formally Lorentz invariant for any choice of the kernel functions. It is easy to see this either by inspection of (11) or by applying infinitesimal Lorentz transformations to (7).

We could have arrived at (7) and (11) also in the following way. Let us assume that we can take the field operators $\varphi(x)$ diagonal, represent the states as functionals of a c -number field $\chi(x)$ which is allowed to vary over the function space \mathfrak{R}^9 and represent the momentum operators by the variational derivative

$$\pi(x) = -i[\delta/\delta\chi(x)]. \quad (14)$$

Then, calling the vacuum functional $\Psi_0(\chi)$ and writing

$$\Psi_0(\chi) = e^{-\Lambda(\chi)}, \quad (15)$$

we immediately get (7). Any other state $\Psi = F(\varphi)\Psi_0$ will be represented by the functional

$$\Psi(\chi) = F(\chi) e^{-\Lambda(\chi)}. \quad (16)$$

Of course, the hard part of the representation problem has not been touched upon by making these assign-

ments for φ and π because one has yet to define the scalar products between states. Alternatively speaking, one must define the process of integration over the space \mathfrak{R} . We will show in the next section that the functional Λ determines the measure of integration, and we shall give formulas for the computation of this measure. Thus the functional Λ occupies a central position in the discussion of the connection between the Hamiltonian and the type of representation of (1). It may be used to characterize the representation and it determines the Hamiltonian by (11).

We now want to mention three simple properties which Λ should possess. The first is obvious: the invariance of the vacuum under the Euclidean group is expressed by

$$\Lambda(\chi) = \Lambda(\chi') \quad \text{with} \quad \chi'(x) = \chi(rx + a), \quad (17)$$

where r is an arbitrary rotation and a an arbitrary translation. Secondly, since $\exp(-\Lambda)$ is essentially the probability amplitude for finding the field $\chi(x)$ in the vacuum state, we expect

$$\lim_{\rho \rightarrow \infty} e^{-\Lambda(\rho\chi)} = 0 \quad (18)$$

for any fixed function χ .

Finally let us imagine a division of space in cells and denote by R_k the set of operators which are functions of the $\varphi(x)$, and $\pi(x)$, with x restricted to the cell k . We shall assume that the Hamiltonian is essentially local, i.e., $H \approx \sum_k H_k$ with H_k belonging to R_k provided the cells are sufficiently large. This means that the projection operator on the vacuum is approximately a product of projections P_k with $P_k \in R_k$. In this approximation $\Psi_0(\chi)$ is then a product of the $\Psi_0(\chi_k)$, where χ_k is the restriction of χ to the cell k , i.e.,

$$\begin{aligned} \chi_k &= \chi(x) & \text{if } x \text{ is in cell } k, \\ \chi_k &= 0 & \text{otherwise.} \end{aligned} \quad (19)$$

Hence

$$\Lambda \approx \sum_k \Lambda(\chi_k). \quad (20)$$

In order to satisfy (20) each kernel function λ_n of a polynomial (12) must tend to zero with increasing distance between any two points x_i and x_j . The advantage of the exponential expression $\Psi_0 = \exp[-\Lambda(\chi)]$ is thus apparent. Indeed, we have here an example of the well known linked cluster expansion which has been used in different forms in statistical mechanics and quantum field theory.¹⁰ The requirement (20) imposes an independent restriction on acceptable choices of mathematically simple functionals $\Psi_0(\chi)$. It would be tempting, for instance, to assume

$$\Psi_0(\chi) = P(\chi) \exp \left[-\frac{1}{2} \int \lambda(x-y) \chi(x) \chi(y) d^3x d^3y \right], \quad (21)$$

⁹ We shall not make any specific assumptions about \mathfrak{R} in this paper except that it shall be a linear space of functions.

¹⁰ See Appendix II for examples and references.

where P is a polynomial of finite degree, since the vacuum expectation values of products of fields could then be evaluated explicitly. However, the requirement (20) rules out such an ansatz.

To close this section we want to make some remarks about the problem of solving Eq. (11) for Λ if H is given. One can set up a Ritz variational principle to determine the "best" bilinear choice for Λ . This leads to a nonlinear integral equation for the kernel function λ (see Appendix III). It is not clear to us, however, under what circumstances such an approximation can be trusted. Alternatively one may set up a systematic perturbation scheme for the calculation of Λ if H' is of polynomial form. One then starts with a bilinear zero-order Hamiltonian

$$H_0' = -\frac{1}{2} \int L^{(0)}(x_1 - x_2) \varphi(x_1) \varphi(x_2) d^3x_1 d^3x_2.$$

Putting $H' = H_0' + gH^I$ one expands the kernel functions λ_n into power series in the coupling constant:

$$\lambda_n = \sum_k g^k \lambda_n^{(k)}.$$

Starting from the zero-order solution,

$$\lambda(p) = [h^{(0)}(p)]^{\frac{1}{2}}, \quad \lambda_n^{(0)} = 0 \quad \text{for } n \neq 2,$$

the calculation is completely straightforward and need not be described here. $h^{(0)}(p)$ is the Fourier transform of $h^{(0)}(x)$. The two approaches could be combined if one takes as the starting point of the perturbation calculation the result of the variational method.

III. THE EXPECTATION FUNCTIONAL

We use the notation

$$\varphi(f) = \int \varphi(x) f(x) d^3x, \quad (22)$$

$$U(f) = \exp i \varphi(f).$$

These quantities are, respectively, Hermitian and unitary operators if f is a real function of x belonging to a space \mathfrak{R}_1 , the test function space. We will not explore the consistency conditions which must be observed in the choice of the spaces \mathfrak{R} and \mathfrak{R}_1 . This question is one of the central points in the mathematical representation theory of the canonical commutation relations (1).^{6,7} Here we shall only assume the existence of the "scalar product"

$$(\chi, f) = \int \chi f d^3x \quad (23)$$

for every $f \in \mathfrak{R}$, and $\chi \in \mathfrak{R}$. We now define the "expectation functional" $E(f)$ by

$$E(f) = (\Psi_0 U(f) \Psi_0) (\Psi_0, \Psi_0)^{-1}. \quad (24)$$

It will be convenient in the following not to normalize Ψ_0 to unity at the outset. $E(f)$ is the generating functional of the vacuum expectation values of field products since

$$E(f) = \sum_n (i^n/n!) \int f(x_1) \cdots f(x_n) \times g_n(x_1 \cdots x_n) d^3x_1 \cdots d^3x_n, \quad (25)$$

with

$$g_n(x_1 \cdots x_n) = (\Psi_0, \varphi(x_1) \cdots \varphi(x_n) \Psi_0) (\Psi_0, \Psi_0)^{-1}. \quad (26)$$

It is sometimes useful to put

$$E(f) = \exp \eta(f), \quad (27)$$

because η has the linked cluster property (20). η is the generating functional for the system of "truncated vacuum expectation values" or " η -functions."¹¹

The functional E may be used to define the scalar product between state vectors in the following manner: According to assumption (ii) every state vector Ψ can be expressed in the form

$$\Psi = F(\varphi) \Psi_0. \quad (28)$$

The scalar product (Ψ_1, Ψ_2) therefore takes the form

$$(\Psi_1, \Psi_2) = (\Psi_0, F_1(\varphi)^* F_2(\varphi) \Psi_0). \quad (29)$$

However, for any functional $F(\varphi)$ we have according to (22)

$$(\Psi_0, F(\varphi) U(f) \Psi_0) = F(-i\delta/\delta f) E(f) (\Psi_0, \Psi_0), \quad (30)$$

and hence

$$(\Psi_0, F(\varphi) \Psi_0) = [F(-i\delta/\delta f) E(f)]_{f=0} (\Psi_0, \Psi_0). \quad (31)$$

The definition of the scalar product implies a definition of a functional integral over the representative functionals (16).

$$(\Psi_0, \Psi_0) = \int e^{-2\Lambda(\chi)} \delta\chi, \quad (32)$$

$$(\Psi_1, \Psi_2) = \int F_1^*(\chi) F_2(\chi) e^{-2\Lambda(\chi)} \delta\chi.$$

For any functional $G(\chi)$ the integral then is defined by

$$\int G(\chi) \delta\chi = (\Psi_0, e^{2\Lambda(\varphi)} G(\varphi) \Psi_0). \quad (33)$$

A functional $G(\chi)$ is integrable if the right-hand side of (33) exists. A sensibly defined integral should be linear and invariant under translations; i.e.,

$$\int [G_1(\chi) + G_2(\chi)] \delta\chi = \int G_1(\chi) \delta\chi + \int G_2(\chi) \delta\chi, \quad (34)$$

¹¹ P. Kristensen, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. 28, No. 17 (1954); E. Freese, Nuovo cimento 2, 50 (1955).

and

$$\int G(\chi + \chi_1) \delta\chi = \int G(\chi) \delta\chi. \quad (35)$$

The relation (34) obviously holds for the definition (33). Equation (35) is also easily verified from

$$\begin{aligned} \int G(\chi + \chi_1) \delta\chi &= (\Psi_0, e^{2\Lambda(\varphi)} G(\varphi + \chi_1) \Psi_0) \\ &= (e^{-i\int \pi(x) \chi_1(x) dx} e^{\Lambda(\varphi)} \Psi_0, \\ &\quad G(\varphi) e^{-i\int \pi(x) \chi_1(x) dx} e^{\Lambda(\varphi)} \Psi_0). \end{aligned} \quad (36)$$

The right hand side of (36) is independent of χ_1 since $\pi \exp \Lambda(\varphi) \Psi_0$ vanishes according to (7) and (8).

We shall make use of (34) and (35) in a heuristic fashion in order to evaluate the functional integrals. Imagine for a moment instead of the functional $G(\chi)$ a function of a finite number of variables $G(q_1 \cdots q_n)$. It is well known that for such functions the properties corresponding to (34), (35) are sufficient to determine the meaning of the integration symbol apart from an arbitrary normalization factor. Let us now take a complete and linearly independent but not necessarily orthogonal basis of functions χ_k in \mathfrak{R} and represent an arbitrary χ by its expansion coefficients q_k in that basis. The functional $G(\chi)$ then becomes a function of the countably infinite set q_k . The analogy with the case of a finite number of q_k would lead us to infer from (34), (35)

$$\int G(\chi) \delta\chi = \text{const} \int G(q_1 q_2 \cdots) dq_1 dq_2 \cdots \quad (37)$$

The right-hand side is still only of symbolic value but it will be given a precise meaning below, at least for some simple cases.

We turn to the problem of computing $E(f)$ from a given Λ . According to (24) and (33) we may write

$$\begin{aligned} E(f) &= \left[\int \exp(-2\Lambda) \delta\chi \right]^{-1} \int \exp[i(\chi, f) - 2\Lambda(\chi)] \delta\chi \\ &= \left\{ \int \exp[-2\Lambda(q_1 q_2 \cdots)] dq_1 dq_2 \cdots \right\}^{-1} \\ &\quad \times \int \exp[i \sum q_k (\chi_k, f) - 2\Lambda(q_1 q_2 \cdots)] dq_1 dq_2 \cdots \end{aligned} \quad (38)$$

In order to evaluate the integrals in (38) we appeal to the linked cluster property of Λ which implies that in a suitable basis Λ is approximately a sum of terms, each of which depends only on a finite number of q_k 's. Let us therefore restrict our attention first to cases in which Λ is of the form

$$\Lambda = \sum_i \lambda(q_i \cdots q_{i+n}). \quad (39)$$

We also restrict ourselves to test functions for which all but a finite number of the (χ_k, f) vanish. This latter

restriction is not serious because, if (38) is meaningful for these special test functions, then the remaining question is one of extending the definitions. In other words, it concerns the precise nature of the test function space which we shall not attempt to discuss in this paper. Under the conditions stated we may write instead of (38)

$$\begin{aligned} E(f) &= \lim_{N \rightarrow \infty} \left\{ \int \exp[-2 \sum_i \lambda(q_i \cdots q_{i+n})] dq_{-N} \cdots dq_N \right\}^{-1} \\ &\quad \times \int \exp\{i \sum_k q_k (\chi_k, f) - 2 \sum_i \lambda(q_i \cdots q_{i+n})\} \\ &\quad \times dq_{-N} \cdots dq_N. \end{aligned} \quad (40)$$

In the sums in (40) the index i shall run from $-(N+n)$ to $+N$ because the contributions which are due to an i outside of this interval cancel. For each N the right-hand side is then well defined. We need to show that the limit exists. We shall do this for an example which brings out most of the points of interest. Take $n=1$ and, for instance,

$$\lambda(q_i, q_{i+1}) = -\frac{1}{2} q_i^4 + \rho q_i q_{i+1} - \frac{1}{2} q_{i+1}^4, \quad (41)$$

and take test functions f for which $(\chi_k, f) = \alpha_k$ for $n_1 \leq k \leq n_2$ and $(\chi_k, f) = 0$ for all other values of k . Then (40) becomes

$$\begin{aligned} E(f) &= \lim [K^{(2N+2)}(q_{-N-1}, q_{N+1})]^{-1} \\ &\quad \times \int K^{(N+n_1+1)}(q_{-N-1}, q_{N+1}) \cdot \exp(i \sum_{k=n_1}^{n_2} \alpha_k q_k) \\ &\quad \times K(q_{n_1}, q_{n_1+1}) \cdots K(q_{n_2-1}, q_{n_2}) K^{(N+1-n_2)}(q_n, q_{N+1}) \\ &\quad \times dq_{n_1} \cdots dq_{n_2}, \end{aligned} \quad (42)$$

where

$$K(q_1 q') = \exp[-2\lambda(q_1 q')],$$

and $K^{(n)}$ is the n -fold iterated kernel. Now we observe that K is a kernel of Hilbert-Schmidt type. Therefore it has a highest eigenvalue κ which is separated by a finite distance from the next eigenvalue. Degeneracy could only be accidental. So we will argue that it is nondegenerate. The eigenfunction to the highest eigenvalue we denote by $\varphi(q)$. As N gets larger only the contribution from the highest eigenvalue survives and we get in the limit

$$\begin{aligned} E(f) &= \kappa^{-(n_2-n_1)} \int \varphi(q_{n_1}) \exp(i \sum_{n_1}^{n_2} \alpha_k q_k) K(q_{n_1}, q_{n_1+1}) \\ &\quad \times \cdots \times K(q_{n_2-1}, q_{n_2}) \varphi(q_{n_2}) dq_{n_1} \cdots dq_{n_2}. \end{aligned} \quad (43)$$

Thus the evaluation of the functional integral is reduced in this case to the eigenvalue problem for the kernel K

and a finite number of integrations. This simple result suggests that, starting from (38) useful approximation procedures may be developed for the calculation of E from Λ also in more realistic cases.

A perturbation theory of the expectation functional can best be developed starting from the definition (24). Let ϕ_0 be a state represented by $\exp[-\Lambda_0(\chi)]$ for which the expectation functional

$$E_0(f) = (\phi_0, U(f)\phi_0)(\phi_0, \phi_0)^{-1} \quad (44)$$

is known explicitly. Such is the case for bilinear Λ_0

$$\Lambda_0(\varphi) = \frac{1}{2} \int \lambda(x_1, x_2) \varphi(x_1) \varphi(x_2) d^3x_1 d^3x_2. \quad (45)$$

We have then

$$E_0(f) = \exp \left[-\frac{1}{4} \int \lambda^{-1}(x_1, x_2) f(x_1) f(x_2) d^3x_1 d^3x_2 \right] \quad (46)$$

$$\equiv \exp \eta_0(f).$$

The vacuum state Ψ_0 can be expressed by

$$\Psi_0 = \exp[-\Lambda'(\varphi)]\phi_0, \quad (47)$$

where $\Lambda' \equiv \Lambda - \Lambda_0$.

The expectation functional $E(f)$ takes the form

$$E(f) = (\phi_0, \exp[-2\Lambda'(\varphi)]U(f)\phi_0) \times (\phi_0, \exp[-2\Lambda'(\varphi)]\phi_0)^{-1}, \quad (48)$$

and hence

$$E(f) = \{ \exp[-2\Lambda'(-i\delta/\delta f')] E_0(f') \}_{f'=0}^{-1} \times \exp[-2\Lambda'(-i\delta/\delta f)] E_0(f). \quad (49)$$

A perturbation expansion for $E(f)$ is obtained by expanding the exponentials. The denominator guarantees the condition $E(0)=1$. To make evident the correspondence between the terms of the perturbation series and diagrams, one may introduce a set of creation and annihilation operators $a^\dagger(x), a(x)$ in a formal Fock space with the formal vacuum Ω_0 . Then, making the substitutions $f(x) \rightarrow -ia^\dagger(x)$, $-i(\delta/\delta f(x)) \rightarrow a(x)$, one gets from (49) the following expressions for the vacuum expectation values (26):

$$g_n(x_1 \cdots x_n) = \langle \Omega_0 | \exp[-2\Lambda'(a)] E_0(-ia^\dagger) | \Omega_0 \rangle^{-1} \times \langle \Omega_0 | a(x_1) \cdots a(x_n) \exp[-2\Lambda'(a)] E_0(-ia^\dagger) | \Omega_0 \rangle. \quad (50)$$

If, as assumed, E_0 is of the form (46) one can simplify the expression by shifting E_0 to the left and obtain

$$g_n(x_1 \cdots x_n) = \langle \Omega_0 | b(x_1) \cdots b(x_n) \exp[-2\Lambda'(b)] | \Omega_0 \rangle \times \langle \Omega_0 | \exp[-2\Lambda'(b)] | \Omega_0 \rangle, \quad (51)$$

with

$$b(x) = a(x) + \frac{1}{2} \int \lambda^{-1}(x, y) a^\dagger(y) d^3y.$$

The evaluation of the numerator clearly leads to Feynman diagrams with the propagator $\frac{1}{2}\lambda^{-1}$ and vertices which are the kernel functions of Λ' . If the numerator and denominator are evaluated separately it is necessary to introduce a finite volume or the equivalent but the ratio is independent of this volume. In fact, if one uses the diagram language one finds that the volume-dependent terms arise from diagrams with disconnected vacuum parts. One can show that one obtains the correct ratio (49) or (50) if one omits all such diagrams in the numerator and drops the denominator at the same time.⁴

We still want to describe a perturbation scheme for the η -functional which is defined by $E(f) = \exp \eta(f)$. This scheme has the advantage that no volume-dependent terms arise at any stage of the calculation. From (49) follows

$$\frac{\delta \eta_0}{\delta f} = e^{-\eta_0(f)} \exp[2\Lambda'(-i\delta/\delta f)] \frac{\delta \eta}{\delta f} \times \exp[-2\Lambda'(-i\delta/\delta f)] e^{\eta_0(f)}. \quad (52)$$

Equation (52) yields a perturbation series for the η -functions in a straightforward manner,

$$\eta = \sum_{n=0}^{\infty} \eta_n,$$

where η_n is determined by the recursion formula

$$\frac{\delta \eta_n}{\delta f} = -e^{-\eta_0} \left\{ [2\Lambda', \delta \eta_{n-1}/\delta f] + \frac{1}{2!} [2\Lambda', [2\Lambda', \delta \eta_{n-2}/\delta f]] + \cdots \right\} e^{\eta_0}. \quad (53)$$

One observes that there exists an exact formal analogy between the problem discussed in this section, namely the computation of $E(f)$ from Λ , and the problem of computing the vacuum expectation values of time-ordered products in a local field theory from the Hamiltonian. Let x now be a space-time point and consider field equations of the form

$$(\square - m^2)\varphi(x) = -\delta \mathcal{L}'/\delta \varphi(x)$$

\mathcal{L}' is the interaction part of the action integral. Furthermore let $\mathcal{T}(f)$ be the generating functional of the system of τ -functions defined by

$$\mathcal{T}(f) = \sum i^n (n!)^{-1} \int f(x_1) \cdots f(x_n) \times \tau(x_1 \cdots x_n) d^4x_1 \cdots d^4x_n, \quad (54)$$

$$\tau(x_1 \cdots x_n) = (\Psi_0, T[\varphi(x_1) \cdots \varphi(x_n)] \Psi_0),$$

where T is the time-ordering symbol. Then the formulas of this section may be literally transcribed according to

the key

space \leftrightarrow space-time,

$$\begin{aligned} E(f) &\leftrightarrow \mathcal{T}(f), \\ -2\Lambda' &\leftrightarrow i\mathcal{E}', \\ -2\Lambda &\leftrightarrow i\mathcal{E}, \end{aligned} \quad (55)$$

$$\mathcal{L} = \frac{1}{2} \int \varphi(x) (\square - m^2) \varphi(x) d^4x + \mathcal{L}'.$$

In this manner (37) goes over into a certain version of the Feynman integral¹²; the counterparts of (49) and the perturbation scheme derived from it are well known.¹³ In spite of this exact formal correspondence there is a decisive difference between the 3-dimensional and the 4-dimensional formalisms. It can be seen from the fact that in the first case the integrands of the functional integrals have the damping factor $\exp(-2\Lambda)$ while in the second case there is an oscillating factor instead. Again, if one uses the 4-dimensional formalism to calculate the equal-time vacuum expectation values, the perturbation series proceeds according to powers of H' whereas in the 3-dimensional formalism this calculation is broken up into the two steps $H \rightarrow \Lambda$ and $\Lambda \rightarrow E$.

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APPENDIX I. MATHEMATICAL SUPPLEMENT

We want to give here a precise mathematical formulation of the basic assumption (ii) of Sec. II and of some of its consequences. Let us consider the set $\{A\}$ of operators which are of the form

$$A = \sum_{i=1}^N c_i U(f_i), \quad (I.1)$$

where N, c_i, f_i are arbitrary. [$\{A\}$ contains all linear combinations of a finite number of $U(f_i)$.] We denote the von Neumann ring which is generated by these operators by \mathfrak{A} . \mathfrak{A} consists of all bounded operators in the representation space which either belong to $\{A\}$ or are strong limits of sequences in $\{A\}$. The precise formulation of our assumption (ii) then is that

$$\mathfrak{A}(\Psi_0) = \mathfrak{D} \quad (I.2)$$

¹² R. P. Feynman, thesis, Princeton, 1942 (unpublished); Revs. Modern Phys. **20**, 367 (1948); J. G. Polkinghorne, Proc. Roy. Soc. (London) **A230**, 272 (1955); P. T. Mathews and A. Salam, Nuovo cimento **2**, 120 (1955); J. Klauder, thesis, Princeton, 1959 (unpublished).

¹³ M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951); F. Coester, Phys. Rev. **95**, 1318 (1954); J. G. Valatin, Proc. Roy. Soc. (London) **229**, 221 (1955).

is a dense set of vectors in the representation space. In standard terminology this is expressed as: Ψ_0 is a cyclic vector with respect to the ring \mathfrak{A} .

The following two statements are consequences:

- (1) If an operator B commutes with \mathfrak{A} and annihilates the vacuum then $B=0$. [Compare (5), Sec. II.]
- (2) \mathfrak{A} is maximal abelian, i.e., every bounded operator which commutes with \mathfrak{A} belongs to \mathfrak{A} . The first statement is easily proved by

$$B\mathfrak{D} = B\mathfrak{A}(\Psi_0) = \mathfrak{A}(B\Psi_0) = 0.$$

The proof of the second statement has been given by Segal.¹⁴ Conversely: If one applies the spectral theorem to the abelian ring \mathfrak{A} one obtains a decomposition of the space into a direct integral

$$\mathfrak{S} = \int \mathfrak{S}^{(\lambda)} d\mu(\lambda), \quad (I.3)$$

such that every operator of the ring acts as a multiple of the identity in each $\mathfrak{S}^{(\lambda)}$. If the ring is *maximal* abelian then the $\mathfrak{S}^{(\lambda)}$ are one-dimensional. In that case every vector which has nonvanishing components in (almost) all $\mathfrak{S}^{(\lambda)}$ is a cyclic vector with respect to \mathfrak{A} . Therefore assumption ii) can be replaced by the requirements that \mathfrak{A} be maximal abelian and that the vacuum state shall have nonvanishing components almost everywhere in the spectral decomposition.

For Eq. (9) in Sec. II the distinction between vanishing "almost nowhere" and vanishing "nowhere" becomes important. Take the example of the single harmonic oscillator. The excited states as well as the ground state are cyclic vectors since the nodes are isolated points which have measure zero. We can therefore go through the argument leading to (9) taking for Ψ_0 the first excited oscillator state. The zero of the energy scale must, of course, be correspondingly adjusted, i.e., we should put then

$$H = \frac{1}{2}(p^2 + q^2) - \frac{3}{2}. \quad (I.4)$$

Arguing as in Sec. II we obtain

$$\begin{aligned} A &= 2^{-\frac{1}{2}}(p - iL), & A^\dagger &= 2^{-\frac{1}{2}}(p + iL), \\ L &= q - q^{-1} & H &= A^\dagger A. \end{aligned} \quad (I.5)$$

The appearance of (I.5) seems in contradiction to the fact that H now has a negative eigenvalue. This apparent paradox is explained as follows: although A^\dagger is formally the Hermitian conjugate of A it is not a proper adjoint because of the singular character of L .¹⁵

APPENDIX II. THE LINKED CLUSTER THEOREM

In statistical mechanics and in quantum field theory one is frequently dealing with hierarchies of the functions $g_n(x_1 \cdots x_n)$ which have the following asymptotic

¹⁴ I. E. Segal, Mem. Am. Math. Soc. **9**, 65 (1951).

¹⁵ We are indebted to V. Bargman and H. Araki for a clarification of this point.

property: If we divide the points $x_1 \cdots x_n$ in an arbitrary fashion into m clusters of $k_1 \cdots k_m$ points, respectively, and denote the points in the i th cluster by $x_{i1} \cdots x_{ik_i}$ then, as we increase the separation between the different clusters

$$g_n(x_1 \cdots x_n) \rightarrow g_{k_1}(x_{11} \cdots x_{1k_1}) g_{k_2}(x_{21} \cdots x_{2k_2}) \cdots \times g_{k_m}(x_{m1} \cdots x_{mk_m}). \quad (\text{II.1})$$

The physical meaning of (II.1) is simple. If the functions can be interpreted as probability distributions then (II.1) states that all correlations decrease with increasing separation in space and that one obtains statistical independence in the limit of infinite separation. We shall call here a system of functions with the asymptotic property (II.1) for short a g -system. Examples: Let Ψ be an arbitrary normalized physical state in one of our models. The two most frequently used ways to represent Ψ are (a) by the set of Fock-space amplitudes and (b) by the set of "covariant wave functions." The former are defined by

$$c_n(x_1 \cdots x_n) = N^{-1} \langle \Omega_0 | a(x_1) \cdots a(x_n) | \Psi \rangle. \quad (\text{II.2})$$

In (II.2) Ω_0 is the "unperturbed vacuum," $a(x_k)$ are "bare particle destruction operators" and N is a normalization factor which depends exponentially on the total volume and is introduced to make the amplitudes finite in the case of infinite volume. The covariant wave functions are defined by

$$\varphi_n(x_1 \cdots x_n) = \langle \Psi_0 | \varphi(x_1) \cdots \varphi(x_n) | \Psi \rangle. \quad (\text{II.3})$$

Both sets of functions are g -systems. The reason for this may be seen most simply in the terminology of Eq. (20) of Sec. II. Since both the actual Hamiltonian and the unperturbed Hamiltonian are approximately decomposed in the form (20), the projection operators on the true and on the unperturbed vacuum are both approximately products of projections which belong to R_k . Secondly, every normalizable physical state becomes equivalent to the true vacuum in the asymptotic regions of space. Finally, the bare particle annihilation operators $a(x)$ are "almost local" in the sense used by Haag.¹⁶

The following theorems are useful in dealing with g -systems.

(1) *Truncated functions.* One introduces the system of functions $s_n(x_1 \cdots x_n)$

$$\begin{aligned} g_1(x) &= s_1(x), \\ g_2(x_1, x_2) &= s_2(x_1, x_2) + s_1(x_1)s_1(x_2) \\ g_3(x_1, x_2, x_3) &= s_3(x_1, x_2, x_3) + s_1(x_1)s_2(x_2, x_3) \\ &\quad + s_1(x_2)s_2(x_1, x_3) + s_1(x_3)s_2(x_1, x_2) \\ &\quad + s_1(x_1)s_1(x_2)s_1(x_3), \quad (\text{II.4}) \\ &\dots \\ g_n(x_1 \cdots x_n) &= \sum s_{k_1}(x_{11} \cdots x_{1k_1}) \cdots s_{k_m}(x_{m1} \cdots x_{mk_m}). \end{aligned}$$

¹⁶ R. Haag, Phys. Rev. **112**, 669 (1958).

Let us call R_n the radius of the smallest sphere enclosing the points $x_1 \cdots x_n$. Then (II.1) is equivalent to the statement

$$s_n(x_1 \cdots x_n) \rightarrow 0 \quad \text{for } R_n \rightarrow \infty. \quad (\text{II.5})$$

We call (II.4) the "Ursell expansion" or "linked cluster expansion."¹⁷

(2) *Generating functionals.* For the following it is convenient to define the constants $g_0=1$ and $s_0=0$. Then to any system of functions we define a generating functional by

$$G(f) = \sum (n!)^{-1} \int g_n(x_1 \cdots x_n) \times f(x_1) \cdots f(x_n) dx_1 \cdots dx_n. \quad (\text{II.6})$$

For a g -system the asymptotic property (II.1) is equivalent to

$$G(f_1 + f_2) \rightarrow G(f_1)G(f_2) \quad (\text{II.7})$$

if the separation between the supports of the two test functions f_1 and f_2 is increased towards infinity. On the other hand, for a system of truncated functions the equivalent of (II.5) is

$$S(f_1 + f_2) \rightarrow S(f_1) + S(f_2). \quad (\text{II.8})$$

The Ursell expansion corresponds to the functional relationship

$$G(f) = \exp S(f). \quad (\text{II.9})$$

For formal calculations it is often useful to insert in (II.6) instead of the c -number test function $f(x)$ a set of formal creation operators $a(x)$ as in (50), (51). G and S are then operators in a Fock space and the functions may be obtained from the generating operators by

$$\begin{aligned} g_n(x_1 \cdots x_n) &= \langle \Omega_0 | a(x_1) \cdots a(x_n) G(a^\dagger) | \Omega_0 \rangle, \\ s_n(x_1 \cdots x_n) &= \langle \Omega_0 | a(x_1) \cdots a(x_n) S(a^\dagger) | \Omega_0 \rangle. \end{aligned} \quad (\text{II.10})$$

(3) *Corollary.* For $f(x)=1$ we get from (II.9) the identity

$$\begin{aligned} 1 + \sum_n (n!)^{-1} \int \cdots \int g_n(x_1 \cdots x_n) dx_1 \cdots dx_n \\ = \exp \left[\sum_n (n!)^{-1} \int \cdots \int s_n(x_1 \cdots x_n) dx_1 \cdots dx_n \right]. \end{aligned} \quad (\text{II.11})$$

If the s_n are translationally invariant functions satisfying Eq. (II.5) then $\int \cdots \int s_n(x_1 \cdots x_n) dx_1 \cdots dx_n$ is proportional to the volume V for large V . In that case the left-hand side of (II.11) becomes therefore equal to $\exp cV$, where c is independent of V . Since the nor-

¹⁷ H. P. Ursell, Proc. Cambridge Phil. Soc. **23**, 685 (1927); J. E. Mayer, J. Chem. Phys. **5**, 67 (1937); B. Kahn and G. E. Uhlenbeck, Physica **5**, 399 (1938).

malization factor in (II.2) is given by

$$N = 1 + \sum_n (n!)^{-1} \int \cdots \int |g_n(x_1 \cdots x_n)|^2 dx_1 \cdots dx_n,$$

and $|g_n|^2$ is also a "g-system," the volume-dependence of N is exponential. (See also reference 4.)

APPENDIX III. VARIATIONAL APPROXIMATION FOR Λ

We want to find the best bilinear approximation for Λ . Let us define "best" as that expression which gives the lowest expectation value for H . Consider the mode

$$\begin{aligned} H = & \frac{1}{2} \int \pi(x)^2 d^3x + \frac{1}{2} \int h^{(2)}(x_1 x_2) \varphi(x_1) \varphi(x_2) d^3x_1 d^3x_2 \\ & + (1/4!) \int h^{(4)}(x_1 \cdots x_4) \varphi(x_1) \cdots \varphi(x_4) \\ & \times d^3x_1 \cdots d^3x_4. \quad (\text{III.1}) \end{aligned}$$

[Compare (3) and (4a).] For bilinear Λ we evaluate easily the expectation value of (III.1) using for instance (7), (8), (31) and (46):

$$\begin{aligned} & (\phi_0, \phi_0)^{-1} (\phi_0, H \phi_0) \\ & = \frac{1}{4} \int \lambda(x_1 x) d^3x + \frac{1}{4} \int h^{(2)}(x, x') \lambda^{-1}(x', x) d^3x' d^3x \\ & + (32)^{-1} \int h^{(4)}(x_1 \cdots x_4) \lambda^{-1}(x_1 x_2) \lambda^{-1}(x_3 x_4) \\ & \times d^3x_1 \cdots d^3x_4. \quad (\text{III.2}) \end{aligned}$$

It is convenient to introduce the reciprocal of the Fourier transform of $\lambda(x, y)$ as the unknown. Therefore

we put

$$\lambda(x, y) = (2\pi)^{-3} \int \rho(p)^{-1} \exp i p(x - y) d^3p. \quad (\text{III.3})$$

Furthermore, let $h^{(2)}(p)$ be the Fourier transform of $h^{(2)}(x, y)$ and

$$K(p, q) = (2\pi)^{-3} \int h^{(4)}(\xi, \eta, \zeta) e^{-i(p\xi + q\eta)} d^3\xi d^3\eta d^3\zeta, \quad (\text{III.4})$$

where $\xi = x_1 - x_2$, $\eta = x_2 - x_3$, $\zeta = x_3 - x_4$, then (III.2) becomes

$$\begin{aligned} (2\pi)^3 V^{-1} (\phi_0, \phi_0)^{-1} (\phi_0, H \phi_0) = & \int [\rho(p)^{-1} + h^{(2)}(p) \rho(p)] d^3p \\ & + \frac{1}{8} \int K(p, q) \rho(p) \rho(q) d^3p d^3q. \quad (\text{III.5}) \end{aligned}$$

V is the total volume of space to which $(\phi_0, H \phi_0)$ must, of course, be proportional. To make (III.5) an extremum ρ must satisfy the integral equation

$$\rho(p)^{-2} = h^{(2)}(p) + \frac{1}{4} \int K(p, q) \rho(q) dq. \quad (\text{III.6})$$

We remark that in the case of the local field theory (3), (4)

$$\begin{aligned} h^{(2)} &= p^2 + m^2, \\ h^{(4)}(\xi, \eta, \zeta) &= g_0 (2\pi)^3 \delta(\xi) \delta(\eta) \delta(\zeta), \\ k(p, q) &= g_0. \end{aligned}$$

In this case (III.6) is solvable and leads just to an infinite mass shift,

$$\begin{aligned} \rho(p) &= (p^2 + M^2)^{-\frac{1}{2}} \\ M^2 &= m^2 + \frac{1}{4} g_0 \int (p^2 + M^2)^{-\frac{1}{2}} d^3p. \quad (\text{III.7}) \end{aligned}$$