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Canonical Quantization

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Abstract. The dynamical variables of a classical system form a Lie algebra $\mathfrak{G}$, where the Lie multiplication is given by the Poisson bracket. Following the ideas of SOURIAU and SEGAL, but with some modifications, we show that it is possible to realize $\mathfrak{G}$ as a concrete algebra of smooth transformations of the functionals Φ on the manifold $\mathfrak{M}$ of smooth solutions to the classical equations of motion. It is even possible to do this in such a way that the action of a chosen dynamical variable, say the Hamiltonian, is given by the classical motion on the manifold, so that the quantum and classical motions coincide. In this realization, constant functionals are realized by multiples of the identity operator. For a finite number of degrees of freedom, n, the space of functionals can be made into a Hilbert space $\mathscr{H}$ using the invariant Liouville volume element; the dynamical variables F become operators $\hat{F}$ in this space. We prove that for any hamiltonian H quadratic in the canonical variables $q_1 \ldots q_n, p_1 \ldots p_n$ there exists a subspace $\mathscr{H}_1 \subset \mathscr{H}$ which is invariant under the action of $\hat{p}_j$, $\hat{q}_k$ and $\hat{H}$, and such that the restriction of $\hat{p}_j, \hat{q}_k$ to $\mathscr{H}_1$ form an irreducible set of operators. Therefore, SOURIAU's quantization rule agrees with the usual one for quadratic hamiltonians. In fact, it gives the Bargmann-Segal holomorphic function realization. For non-linear problems in general, however, the operators $\hat{p}_j$, $\hat{q}_k$ form a reducible set on any subspace of $\mathscr{H}$ invariant under the action of the Hamiltonian. In particular this happens for $H = \frac{1}{2} p^2 + \lambda q^4$. Therefore, SOURIAU's rule cannot agree with the usual quantization procedure for general non-linear systems.

The method can be applied to the quantization of a non-linear wave equation and differs from the usual attempts in that (1) at any fixed time the field and its conjugate momentum may form a reducible set (2) the theory is less singular than usual.

For a particular wave equation $(\Box + m^2)\,\phi(x) = \lambda\,\phi^3(x)$, we show heuristically that the interacting field may be defined as a first order differential operator acting on c^∞-functions on the manifold of solutions. In order to make this space into a Hilbert space, one must define a suitable method of functional integration on the manifold; this problem is discussed, without, however, arriving at a satisfactory conclusion.

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1. Introduction

In order to answer the question, is there a quantized field $\phi(x)$ satisfying the equation

$$(\Box + m^2)\, \phi(x) = \lambda\, \phi^3(x)\,, \tag{1}$$

one must first make two definitions.

(a) What is a quantized field? That is, within what class of mathematical objects should we look for solutions?

(b) When may a quantized field, as understood in a definite sense, be said to satisfy (1)?

The best approach to these questions is still very much a matter of opinion. There are several well-developed mathematical frameworks [1], [2], [3], [4], [5], [6] any one of which might be chosen as the answer to (a). Although closely related to each other, these frameworks differ in technical details. It is time to give consideration to question (b), which has received comparatively little attention.

For a wide class of systems with a finite number of degrees of freedom, Souriau [7], [8] has defined what he means by the quantized form of the classical theory, and has found a solution to the problem posed. Although Souriau's quantization procedure differs from the usual one for non-linear systems (as we show) it is adapted here and applied to the quantization of fields. Our treatment is heuristic; however, much of it can be made completely rigorous for the particular classical system defined by equation (1), as shown by Segal [9], [10]; in spirit it is similar to that of Segal in his paper "Explicit formal construction of non-linear quantum fields" [11], [12], although the details differ considerably.

The first part of the problem is to set up the classical theory in a sufficiently convenient form. It turns out to be best expressed in terms of differentiable manifolds (see the book by Sternberg [3]). For a system described by a given Hamiltonian, a *classical path* ϕ is uniquely determined by the values of the dynamical variables $(q_1, \ldots, q_n, p_1, \ldots, p_n)$ at time $t = 0$ say (or any other specified time); the set $\mathfrak{M}$ of solutions ϕ to the classical equations of motion is thus completely parametrized by points in phase space $\mathfrak{H} = \mathbf{R}^n \oplus \mathbf{R}^n$. In the terminology of mathematicians, $\mathfrak{M}$ is a manifold modelled on $\mathfrak{H}$. Instead of using the coordinates $(p, q) \in \mathbf{R}^n \oplus \mathbf{R}^n$ one could use any $2n$ independent functions of them to determine the solution. If we restrict our attention to changes of coordinates defined by infinitely differentiable functions, $\mathfrak{M}$ becomes a c^∞-manifold.

Of great importance is the change of coordinates due to the classical time-evolution. The vector $\{p_1(o), \ldots, p_n(o), q_1(o), \ldots, q_n(o)\}$ becomes the vector $\{p_1(t), \ldots, p_n(t), q_1(t), \ldots, q_n(t)\}$. This is a mapping $\mathfrak{M} \to \mathfrak{M}$. We shall assume that it is a c^∞-mapping.

A *dynamical variable* F is a c^∞-functional on $\mathfrak{M}$; that is, a mapping that assigns to each classical solution $\phi \in \mathfrak{M}$ a complex number $F(\phi)$ such that when we parametrize $\mathfrak{M}$ by $\mathfrak{H}$ in any c^∞-system of coordinates, then F is a c^∞-function of $(q_1, \ldots, q_n, p_1, \ldots, p_n)$. The dynamical variables form a Lie algebra $\mathfrak{G}$; the bracket $\{\ ,\ \}$ is the Poisson bracket defined as

$$\{F, G\} = \sum_{k=1}^{n} \left(\frac{\partial F}{\partial q_k} \frac{\partial G}{\partial p_k} - \frac{\partial F}{\partial p_k} \frac{\partial G}{\partial q_k} \right).$$

The function $\{F, G\}$ is clearly a c^∞-function. SOURIAU defines a quantization of a given classical system $\mathfrak{G}$ to be a representation of $\mathfrak{G}$ by self-adjoint operators on a Hilbert space $\mathscr{H}$ which maps the unit constant functional into $\hbar \mathbf{1}$, where $\mathbf{1}$ is the unit operator in $\mathscr{H}$. By a representation of $\mathfrak{G}$ we mean a solution to the "Dirac Problem" namely, to find a map $F \to \hat{F}$ such that

$$\text{I} \qquad \widehat{\{F, G\}} = i\,[\hat{F}, \hat{G}]_- \tag{2}$$
$$\text{II} \qquad \hat{1} = \hbar \mathbf{1}$$

where $\hat{F}, \hat{G} \ldots$ are operators on $\mathscr{H}$. We note the following differences compared with the usual formulation of the problem.

(1) The usual formulation requires the canonical variables (q, p) to be irreducibly represented, while the Dirac problem does not require this.

(2) In the usual formulation no prescription $F \to \hat{F}$ for assigning operators for the whole of $\mathfrak{G}$ is attempted; certain dynamical variables, including (p, q), are selected for representation. Other dynamical variables may be expressible as operator functions of $\hat{p}$ and $\hat{q}$, but this may not be possible in a way consistent with the Dirac problem.

This difference may be expressed roughly as follows [14]. Normally, one quantizes (p, q) and then solves the operator equation of motion; in the Dirac problem one first solves the classical equation for $(p(t), q(t))$ and then quantizes the result.

SOURIAU obtains the following solution to the Dirac problem; the Hilbert space $\mathscr{H}$ is given by the set of square integrable functions ψ on the manifold $\mathfrak{M}$, that is, on phase space. For any dynamical variable F, the operator $\hat{F}$ is the following first order differential operator:

$$(\hat{F}\psi)(p, q) = \left(F - \sum^{n} p_j \frac{\partial F}{\partial p_j} \right) \psi(p, q) - i\{F, \psi\}(p, q) \tag{3}$$

It is an elementary exercise to show that (3) solves the Dirac problem (2). As it stands, the solution depends on the choice of coordinates, since $\sum^{n} p_j \frac{\partial F}{\partial p_j}$ is not invariant under canonical transformations. The quantization $F \to \hat{F}$ using (3) in some other canonical coordinate system, say $(P_1, \ldots, P_n, Q_1, \ldots, Q_n)$, is unitary equivalent to the one obtained using $(p_1, \ldots, p_n, q_1, \ldots, q_n)$. The proof uses the fact that the scalar product

$$\langle \psi, \varphi \rangle = \int \bar{\psi}(p_1, \ldots, q_n)\, \varphi(p_1, \ldots, q_n)\, dp_1\, dq_1, \ldots, dp_n\, dq_n \tag{4}$$

is invariant under canonical transformations. In order to adapt Eq. (3) to field theory, one must show that the set of solutions to the classical equations has the structure of a differentiable manifold. We note that [9], [10] for Eq. (1) there is a unique, global solution with given values of $\phi(x, t)$ and $\dot{\phi}(x, t)$ on a spacelike surface σ, where these functions are chosen in $\mathscr{D}$. The pair of functions $(\phi(x, t), \phi(x, t))$, defined on a given σ, is called the Cauchy data for the solution. The phase space $\mathfrak{H}$ of the system is the set of Cauchy data, in this case a pair of function spaces $\mathscr{D}(\mathbf{R}^3) \oplus \mathscr{D}(\mathbf{R}^3)$ which can be completed in various ways to form Banach spaces.

A solution is also determined by its values on a different space-like surface σ'. It can be proved that if the Cauchy data on σ are c^∞-functions of compact support, the same holds on any other space-like surface. In fact, the disturbance propagates smoothly at velocities up to the speed of light, by the hyperbolic character of the equation. The transformation $\sigma \to \sigma'$ thus defines a transformation $\mathfrak{H} \to \mathfrak{H}$, i.e. a change of coordinates. For Eq. (1) this is a c^∞-change. (For a simple definition of c^∞-functions on any topological space, see LANG [15].) Thus the class of solutions under discussion does form a manifold, $\mathfrak{M}$ say. Just as before, one may define the classical Lie algebra $\mathfrak{G}$ of the system as the set of c^∞-functionals on the manifold, furnished with the Poisson bracket. In order that the Poisson bracket be defined, present results for Eq. (1) would have to be extended somewhat, so that the spaces of Cauchy data in ϕ and $\dot{\phi}$ are dual pairs, say $\phi \in \mathscr{B}$ and $\dot{\phi} \in \mathscr{B}'$. For then if $F(\phi, \dot{\phi})$ is a c^∞-functional, $\frac{\delta F}{\delta \phi}$ is in $\mathscr{B}'$ and $\frac{\delta F}{\delta \dot{\phi}}$ is in $\mathscr{B}'' = \mathscr{B}$, and the bracket

$$\{F, G\} = \left\langle \frac{\delta F}{\delta \phi}, \frac{\delta G}{\delta \dot{\phi}} \right\rangle - \left\langle \frac{\delta F}{\delta \dot{\phi}}, \frac{\delta G}{\delta \phi} \right\rangle, \tag{5}$$

becomes well defined. It is legitimate in this case to use the common notation for distributions

$$\{F, G\} = \int d^3x \frac{\delta F}{\delta \phi(\mathbf{x}, 0)} \frac{\delta G}{\delta \dot{\phi}(\mathbf{x}, 0)} - \int d^3x \frac{\delta F}{\delta \dot{\phi}(\mathbf{x}, 0)} \frac{\delta G}{\delta \phi(\mathbf{x}, 0)}\,. \tag{6}$$

It turns out that our eventual suggestion for the quantized field, Eq. (53), is well defined even without this extension of known results.

Thus, in attempting to treat field theory by SOURIAU's method, one can get as far as Eq. (3) without serious trouble. The real difficulty comes when we try to write down the scalar product (4) for infinitely many degrees of freedom, since the canonically invariant volume element

$\prod_{j=1}^{j=\infty} dp_j\, dq_j$ no longer has a meaning. This would have to be replaced by a functional integral (10); assuming that a suitable scalar product can be defined we get a Hilbert space $\mathscr{H}$ and operators $\hat{\phi}$ on $\mathscr{H}$ given by Eq. (3). We shall then say that $\hat{\phi}(x)$ „satisfies Eq. (1)". The sense in which this is so differs from the so-called usual one (which is singular) in that the right hand side of (1) is quantized according to $\widehat{j(x)} = \lambda\, \widehat{\phi^3}(x)$, and this is not equal to $\lambda(\hat{\phi}(x))^3$. However, Eq. (1) holds in a derivative sense; for we have

$$[[\hat{j}(\mathbf{x}, t), \hat{\dot{\phi}}(\mathbf{y}, t)], \hat{\dot{\phi}}(\mathbf{z}, t)] = 6\lambda\, \hat{\phi}(\mathbf{x}, t)\, \delta^3(\mathbf{x} - \mathbf{y})\, \delta^3(\mathbf{x} - \mathbf{z}) \qquad (7)$$

holding, since this is a Lie algebra relation in $\mathfrak{G}$. It was suggested by SEGAL [11], [12] that (7) should replace (1) as the equation of motion. If $(\hat{\phi}(\mathbf{x}, t), \hat{\dot{\phi}}(\mathbf{y}, t))$ forms an irreducible set for fixed time t, (7) implies that $\hat{j}(x, t)$ differs from the usual $\lambda(\hat{\phi}(x))^3$ by terms like $a\, \hat{\phi}(x) + b$ which are interpreted as renormalization terms. We shall see that in the case of a finite number of degrees of freedom, the canonical operators at sharp time in general must be taken to form a reducible set if they are quantized according to SOURIAU. Thus we might expect a similar reducibility to occur in field theory.

In the present paper, we give a heuristic discussion of the program derived from SOURIAU's rule. In Section 2 we show that for quadratic Hamiltonians complete agreement with the usual quantization rules can be obtained by restricting attention to suitable subspaces of square-integrable functions on phase-space. We arrive at the MOYAL-BARGMANN formalism [17], [18], [19] for the harmonic oscillator in terms of anti-holomorphic functions. For a particle with λq^4 interaction, SOURIAU's rule definitely disagrees with the usual rules.

In Section (3) we find the most general linear differential operator solving the Dirac problem, and show that it can be obtained from SOURIAU's rule by a canonical transformation. Using the generalization we construct a quantization rule, unitarily equivalent to SOURIAU's, in which the quantum motion coincides with that given by the classical path in phase space. Applied to field theory one obtains a natural realization of the field operators on the space of functionals of the classical incoming field.

In Section (4) we tentatively suggest how theories with Fermions might be included in the formalism; only gauge invariant quantities can be quantized by this method.

In Section (5) we discuss the problem of functional integration. We show that by quantizing the incoming free field one can allways find a

Lorentz invariant method of functional integration, which however, is not likely to lead to a theory with positive energy. Solving the latter problem is difficult and no simple method suggests itself.

2. Comparison with the usual quantization

SOURIAU's rule (2), as it stands, differs from the usual quantization rule. For the operators $\hat{p}$, $\hat{q}$ are

$$\hat{p} = i\frac{\partial}{\partial q}, \quad \hat{q} = q - i\frac{\partial}{\partial p} \tag{8}$$

and these are reducible on $\mathscr{L}^2(\mathbf{R}^2)$. For example, the operators $p + i\frac{\partial}{\partial q}$ and $i\frac{\partial}{\partial q}$ commute with them. In order to compare with the usual procedure, one must ask if there exists a subspace or differential subspace $\mathscr{H}_1$ of $\mathscr{L}^2(\mathbf{R}^2)$ with the following properties (ignoring domain questions) (i) $\mathscr{H}_1$ is mapped into itself by $\hat{H}$ (ii) $\hat{p}$ and $\hat{q}$ map $\mathscr{H}_1$ into itself and form an irreducible set of operators on $\mathscr{H}_1$.

In his discussion [14] of a suggestion of SEGAL, PROSSER does not consider the question of the reducibility of the canonical operators; SOURIAU [7], [8] suggests an appropriate restriction for certain simple cases, but does not formulate the general problem in the above terms. Conditions (i) and (ii) are necessary and sufficient for SOURIAU's theory, restricted to $\mathscr{H}_1$, to be entirely equivalent to the usual theory, at least for polynomial interactions. We shall show that such a subspace can be found if the Hamiltonian is at most quadratic in the p's and q's, but does not exist for the general non-linear system. We illustrate this by considering the two cases $H = p^2 + q^2$ and $H = \frac{1}{2}p^2 + \lambda q^4$ in detail.

Harmonic Oscillator $H = p^2 + q^2$.

Instead of the rule (3), one may use the formula

$$(\hat{F}\psi)(p,q) = \left(F(p,q) - \frac{1}{2}p\frac{\partial F}{\partial q} - \frac{1}{2}q\frac{\partial F}{\partial p}\right) - i\{F, \psi\} \tag{9}$$

which is rather more symmetrical in p and q. It is easy to see that (9) also solves the Dirac problem; it is obtained from (3) by a linear canonical transformation, and leads to operators that are unitarily related to those obtained by (3). It is clear that the question at issue, whether or not there is a subspace satisfying (i) and (ii), is not affected by a unitary transformation of all the variables, and so we might as well choose the most convenient quantization rule.

The rule (9) assigns to p the operator

$$\hat{p} = \frac{p}{2} + i\frac{\partial}{\partial q} \tag{10}$$

and to q the operator

$$\hat{q} = \frac{q}{2} - i\frac{\partial}{\partial p}\,. \tag{11}$$

These are the same as the quantization rules given by BARGMANN [18], MOYAL [19] and KLAUDER [20], and used by SEGAL for field theory [11], [12], [17]. Rule (9) quantizes the Hamiltonian according to

$$H\psi = -i\{H, \psi\} \tag{12}$$

since $H = p^2 + q^2$ is a homogeneous quadratic function of the variables p and q. For then, by EULER's theorem on homogeneous functions,

$$H - \frac{1}{2}p\frac{\partial H}{\partial p} - \frac{1}{2}q\frac{\partial H}{\partial q} = 0$$

and (9) reduces to (12). Therefore

$$\hat{H} = 2i\left(p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p}\right) = \left(\frac{p}{2} + i\frac{\partial}{\partial q}\right)^2 + \left(\frac{q}{2} - i\frac{\partial}{\partial p}\right)^2 - \left(\frac{p}{2} - i\frac{\partial}{\partial q}\right)^2 - \left(\frac{q}{2} + i\frac{\partial}{\partial p}\right)^2.$$

Let us write $\mathring{H} = \left(\frac{p}{2} + i\frac{\partial}{\partial q}\right)^2 + \left(\frac{q}{2} - i\frac{\partial}{\partial p}\right)^2 = \hat{p}^2 + \hat{q}^2$, which is the usual quantization of the Hamiltonian. Then $\hat{H} - \mathring{H} = -\left(\frac{p}{2} - i\frac{\partial}{\partial q}\right)^2 - \left(\frac{q}{2} + i\frac{\partial}{\partial p}\right)^2$ commutes with $\hat{p}$ and $\hat{q}$. Therefore, restricting all the operators to the subspace $\mathscr{H}_1$ on which $\hat{p}$ and $\hat{q}$ are irreducible, there must exist a number, say E_0, such that for all $\psi \in \mathscr{H}_1$

$$(\hat{H} - \mathring{H})\,\psi = E_0\psi\,,$$

that is

$$\left(\frac{p}{2} - i\frac{\partial}{\partial q}\right)^2\psi + \left(\frac{q}{2} + i\frac{\partial}{\partial p}\right)^2\psi + E_0\psi = 0\,. \tag{14}$$

Equation (14) is a second order differential equation that must be satisfied by the vectors of any subspace $\mathscr{H}_1$ satisfying (i) and (ii). Conversely the set of solutions of (14) is invariant under $\hat{p}$ and $\hat{q}$, and therefore under $\hat{H}$ and $\mathring{H}$. To see this note that

$$(\hat{H} - \mathring{H} - E_0)\,\hat{p}\psi = [\hat{H} - \mathring{H} - E_0, \hat{p}]\,\psi + \hat{p}(\hat{H} - \mathring{H} - E_0)\psi = 0 \quad \text{for} \quad \psi \in \mathscr{H}_1\,.$$

Similarly $\hat{q}\psi$ is also a solution of (14) if ψ is, and therefore $(\hat{p}^2 + \hat{q}^2)\psi$ is also a solution. But on $\mathscr{H}_1$, $\hat{H}$ coincides with $\mathring{H}$, proving that $\hat{H}\psi \in \mathscr{H}_1$ for any $\psi \in \mathscr{H}_1$.

We have yet to show that we may choose a subset of solutions to (15) that are square-integrable and whose closure forms a non-trivial space on which $\hat{p}$ and $\hat{q}$ are irreducible. With an eye to the answer, write

$\psi = e^{-\frac{1}{4}(p^2+q^2)}\varphi$. Substituting in Eq. (14), and simplifying, we find

$$\frac{\partial^2 \varphi}{\partial p^2} + \frac{\partial^2 \varphi}{\partial q^2} - (p + iq)\frac{\partial \varphi}{\partial p} + (p + iq)\, i \frac{\partial \varphi}{\partial q} - \varphi = E_0 \varphi \qquad (15)$$

Putting $z = p + iq$, $\bar{z} = p - iq$, this equation is

$$\frac{\partial}{\partial \bar{z}} \frac{\partial \varphi}{\partial z} - z \frac{\partial \varphi}{\partial z} = (E_0 + 1)\, \varphi\,. \qquad (16)$$

A solution to (16) is $\frac{\partial \varphi}{\partial z} = 0$, $E_0 = -1$; thus we may take the subspace $\mathscr{H}_1$ of $\mathscr{L}^2(\mathrm{R}^2)$ to consist of anti-holomorphic functions φ, integrable with respect to the scalar product

$$(\varphi_1, \varphi_2) = \int e^{-\frac{1}{2}(p^2+q^2)}\, \bar{\varphi}_1\, \varphi_2\, dp\, dq\,.$$

We have therefore arrived at the representation of the harmonic oscillator by anti-holomorphic functions in the complex plane; as proved in detail by BARGMANN [18], this is entirely equivalent to the usual theory.

Looking at Eq. (13) we see that the restriction to the subspace $\mathscr{H}_1$ not only makes $\hat{p}$ and $\hat{q}$ irreducible, but is a direct way to eliminate the negative energies that would arise from the negative sum of squares in (13).

Non-linear Problem $H = \frac{1}{2} p^2 + \lambda q^4$.

Let us quantize this theory using Eq. (3); thus

$$\hat{p} = i \frac{\partial}{\partial q}\,, \quad \hat{q} = q - i \frac{\partial}{\partial p}$$

and

$$\hat{H} = \left(\frac{-p^2}{2} + \lambda q^4\right) - 4i\,\lambda q^3 \frac{\partial}{\partial p} + ip \frac{\partial}{\partial q}\,. \qquad (17)$$

We will show there is no subspace $\mathscr{H}_1$ satisfying (i) and (ii). Let us write

$$\mathring{H} = \frac{1}{2}(\hat{p})^2 + \lambda(\hat{q})^4 \qquad (18)$$

which is the "usual" quantization of this system. It is clear that any subspace $\mathscr{H}_1$ invariant under $\hat{p}$ and $\hat{q}$ will also be invariant undet $\mathring{H}$. We remark that since (3) solves the Dirac problem, and $[\hat{p}, [\hat{p}, \hat{H}]]$ is linear in $\hat{q}$, we must have $[\hat{p}, [\hat{p}, \hat{H} - \mathring{H}]] = 0$. Further, $\hat{H} - \mathring{H}$ commutes with $\hat{q}$. Since by assumption, $\hat{H}$, and therefore $\hat{H} - \mathring{H}$, maps $\mathscr{H}_1$ into itself, the restriction of $\hat{H} - \mathring{H}$ to $\mathscr{H}_1$ must be a function of $\hat{q}$ restricted to $\mathscr{H}_1$, since this operator is a complete commuting set when restricted. Since $\hat{p}$ and $\hat{q}$ are irreducible on $\mathscr{H}_1$, the equation $[\hat{p}, [\hat{p}, \hat{H} - \mathring{H}]] = 0$ implies that $\hat{H} - \mathring{H}$ is at most a quadratic function of $\hat{q}$ when restricted. It follows that vectors in $\mathscr{H}_1$, if it exists, must satisfy the fourth order differential equation

$$(\hat{H} - \mathring{H} - \alpha \hat{q}^2 - \beta \hat{q} - \gamma)\psi = 0 \qquad (19)$$

for some numbers α, β and γ, which may be interpreted as renormalization constants.

The set of solutions to (19) is not invariant under the action of $\hat{p}$, and so vectors in $\mathscr{H}_1$ are subject to the further condition

$$(\hat{H} - \mathring{H} - \alpha\hat{q}^2 - \beta\hat{q} - \gamma)\,\hat{p}\psi = 0\,.$$

For vectors in $\mathscr{H}_1$ this is equivalent to

$$[(\hat{H} - \mathring{H} - \alpha\hat{q}^2 - \beta\hat{q} - \gamma), \hat{p}]\psi = 0$$

which simplifies to

$$-4i\lambda\left(3q\frac{\partial^2\psi}{\partial p^2} + i\frac{\partial^3\psi}{\partial p^3}\right) + 2i\alpha\left(q\psi - i\frac{\partial\psi}{\partial p}\right) + i\beta\psi = 0\,. \tag{20}$$

The set of simultaneous solutions to (19) and (20) is again not invariant under the action of $\hat{p}$, and so vectors in $\mathscr{H}_1$ satisfy the further independent condition

$$(\hat{H} - \mathring{H} - \alpha\hat{q}^2 - \beta\hat{q} - \gamma)\,\hat{p}^2\psi = 0\,.$$

For solutions to (19) and (20) this may be written as

$$[[(\hat{H} - \mathring{H} - \alpha\hat{q}^2 - \beta\hat{q} - \gamma), \hat{p}], \hat{p}] = 0 \tag{21}$$

which reduces to

$$-12\lambda\frac{\partial^2\psi}{\partial p^2} + 2\alpha\psi = 0\,. \tag{22}$$

The conditions (20) and (22) are equivalent to the constraint

$$\alpha^3 = \frac{-27}{32}\beta^2 \tag{23}$$

and the condition

$$\frac{\partial\psi}{\partial p} = \frac{-3i}{8}\frac{\beta}{\alpha}\psi\,. \tag{24}$$

We learn from (24) that the p-dependence of any $\psi \in \mathscr{H}_1$ is essentially trivial. But such a form cannot possibly satisfy Eq. (19), which contains the multiplication operator $-\frac{1}{2}p^2$. We conclude that for this system there does not exist a subspace $\mathscr{H}_1$ with the desired properties.

There is another, more general sense in which one may say that our quantization "agrees" with the usual one. In this new sense one does not demand that the subspace $\mathscr{H}_1$ be mapped into itself by the Hamiltonian; one demands only that the time development of the operators $\hat{p}$ and $\hat{q}$ as given by $\widehat{p(t)}$, $\widehat{q(t)}$, is the same automorphism of the ring generated by $\widehat{p(o)}$, $\widehat{q(o)}$ (restricted to $\mathscr{H}_1$) as is given by the usual theory, up to harmless renormalization terms. More specifically, we might seek a subspace $\mathscr{H}_1'$ with the properties

(i) For each t, $\widehat{p(t)}$ and $\widehat{q(t)}$ map $\mathscr{H}_1'$ into itself

(ii) For each t, $\widehat{p(t)}$ and $\widehat{q(t)}$ form an irreducible set of operators. However, there is no $\mathscr{H}_1'$ with these properties, and we must be content with the conclusion that for certain interesting elementary systems, SOURIAU's rule gives answers different from the usual one. The details of the more general notion of agreement, using $\mathscr{H}_1'$, are as follows. We require that $\widehat{p(t)}$ and $\widehat{q(t)}$ map $\mathscr{H}_1'$ into itself for all time, and so the time derivatives $\widehat{\dot{p}(t)}$, $\widehat{\dot{q}(t)}$ must also have this property, that is $[\hat{H}, \hat{p}]$ and $[\hat{H}, \hat{q}]$ have restrictions to $\mathscr{H}_1'$. But then using the fact that $(\hat{p}, \hat{q})$ are irreducible as before, but with $[\hat{H}, \hat{p}]$ replacing $\hat{H}$ in the argument, one finds that

$$[\hat{H}, \hat{p}] - [\mathring{H}, \hat{p}] = 2\alpha\hat{q} + \beta \tag{25}$$

on $\mathscr{H}_1'$. This leads to Eq. (20). The supposed invariance of $\mathscr{H}_1'$ under the action of $\hat{p}$ leads again to Eq. (22), and so the p-dependence of ψ must be essentially trivial. But this holds for all t, impossible since in general $q(t)$ is a non-trivial function of both $p(0)$ and $q(0)$. This concludes our discussion of (i) and (ii) and the non-linear problem. In this discussion the very special nature of the quadratic Hamiltonian is apparent; for this system the operators $\hat{H}$, $\hat{p}$, $\hat{q}$ and $\mathbf{1}$ form a finite dimensional Lie algebra with $\hat{H}$ acting as an outer derivation of the "Heisenberg algebra" $(\hat{p}, \hat{q}, \mathbf{1})$. Because of this, the solutions to Eq. (16) are mapped into themselves by $\hat{p}$ and $\hat{q}$. For the non-linear problem, this does not happen, and one is led to too many conditions.

For a general system, the path determined by the infinitesimal change

$$\psi \to \psi + \{H, \psi\}$$

is the classical path in the space of functions ψ; that is, the path

$$\{\psi_t = \psi(p(t), q(t)), \quad -\infty < t < \infty\} .$$

The generator is called the *Koopman Hamiltonian* for the problem. We shall call the path determined by

$$\psi \to \psi + i\hat{H}\psi$$

the *Souriau path*, and the path determined by

$$\psi \to \psi + i\mathring{H}\psi$$

the *quantum path*. Thus, when we quantize using (9), the classical path coincides with the Souriau path if and only if H is homogeneous quadratic, and when one restricts to solutions of (16) both paths coincide with the quantum path. This is a well-known result in other terms; in the language of KLAUDER [20], quadratic Hamiltonians possess a quantization in which they are *exact*.

The fact that the classical and Souriau paths coincide for this case is not a significant property of quadratic Hamiltonians. We shall see later that any Hamiltonian possesses a quantization on phase space in which the classical and SOURIAU paths coincide, without, however, being exact, since the quantum path is different.

We note that the SOURIAU and quantum paths depend on the coordinates used in the definitions of $\hat{p}$ and $\hat{q}$ and $\hat{H}$.

Although the difference between the SOURIAU solution and the usual quantum solution is disappointing, it does not exclude the method from being useful in quantum field theory; there, the usual method leads to divergences, while SOURIAU's formula promises to give a field theory with some interesting properties.

3. Effect of a contact transformation

How general is the solution (3) to the Dirac problem? More specifically, one might ask for a solution in terms of finite-order differential operators on phase space of the form

$$\hat{F}\psi = F\psi + \sum_{0 \leq i,j,l,m}^{N} \frac{\partial^{i+j} F}{\partial p^i \partial q^j} f_{i,j,l,m}(p, q) \frac{\partial^{l+m}\psi}{\partial p^l \partial q^m} \tag{26}$$

for some functions $f_{i,j,l,m}$ on phase space (for simplicity we have considered only one degree of freedom). Let us now impose the condition

$$\widehat{\{F, G\}}\, \psi \equiv i(\hat{F}\hat{G} - \hat{G}\hat{F})\psi \tag{27}$$

as an identity in F, G, ψ and all their derivatives. It is likely that the only solution to (27) of the form (26) is actually of first order, namely

$$\begin{aligned} \hat{F}\psi = \Big(F - \frac{1}{2} p \frac{\partial F}{\partial p} - \frac{1}{2} q \frac{\partial F}{\partial q} + f(p, q)F + g(p, q) \frac{\partial F}{\partial p} + \\ + h(p, q) \frac{\partial F}{\partial q}\Big) \psi - i\{F, \psi\} \end{aligned} \tag{28}$$

for some functions f, g and h. The author has proved (by an elementary but lengthy calculation) that (28) follows from (26) and (27) if the sum in (26) is restricted to $i, j, l, m \leq 2$. If we put

$$\alpha(F) = f(p, q)F + g(p, q) \frac{\partial F}{\partial p} + h(p, q) \frac{\partial F}{\partial q} \tag{29}$$

it is easy to see that (27) implies

$$\alpha(\{F, G\}) = \{F, \alpha(G)\} + \{\alpha(F), G\}\,. \tag{30}$$

That is, the mapping $F \to \alpha(F)$ is a *derivation* of the Lie algebra of Poisson brackets. The typical derivation is

$$\alpha(F) = \{W, F\} \tag{31}$$

for some function W of (p, q), and we can easily see that this is the most general form for α satisfying (29) and (30) identically in F and G. In fact, simple substitution of (29) in (30) leads to the equations $f = \text{const}$, $\frac{\partial g}{\partial p} = -\frac{\partial h}{\partial q}$ when we identify the coefficients of F, G, $\frac{\partial F}{\partial p}$, $\frac{\partial F}{\partial q}$ etc. on both sides of the resulting equation. The value of f must be zero if we wish to maintain $\hat{1} = \hbar \mathbf{1}$ where $\mathbf{1}$ is the unit operator[1]. It follows that there exists a function $W(p, q)$ such that $g = \frac{\partial W}{\partial q}$, $h = \frac{\partial W}{\partial p}$ and we are led to (31).

For any function W, provided it is smooth, we get the solution to the Dirac problem

$$\hat{F}\psi = \left(F - \frac{1}{2} p \frac{\partial F}{\partial p} - \frac{1}{2} q \frac{\partial F}{\partial q} + \{W, F\}\right)\psi - i\{F, \psi\}\,. \tag{32}$$

It might be thought that (32) is significantly more general than (3) or (9); but in fact (32) can be obtained from (9) by a canonical transformation, and W is the classical generating function for the transformation. To see this, note that (3) and (9) are not invariant under a change of coordinates. In this discussion we regard the states ψ as functions on the manifold $\mathfrak{M}$, numerically unchanged by a change in coordinates. Similarly the dynamical variables are functions on $\mathfrak{M}$. Thus, the only terms in the two quantization rules

$$\hat{F}\psi = \left(F - p_0 \frac{\partial F}{\partial p_0}\right)\psi - i\{F, \psi\} \tag{33}$$

and

$$\hat{F}'\psi = \left(F - p \frac{\partial F}{\partial p}\right)\psi - i\{F, \psi\} \tag{34}$$

that differ, if $(p_0, q_0) \to (p, q)$ is a canonical transformation, are the second ones, since

$$p_0 \left.\frac{\partial F(p_0, q_0)}{\partial p_0}\right|_{q_0} \neq p(p_0, q_0) \left.\frac{\partial F(p_0(p, q), q_0(p, q))}{\partial p}\right|_{q}\,.$$

In fact

$$p \frac{\partial F(p_0(p, q), q_0(p, q))}{\partial p} = p(p_0, q_0) \frac{\partial F}{\partial p_0} \frac{\partial p_0}{\partial p} + p(p_0, q_0) \frac{\partial F}{\partial q_0} \frac{\partial q_0}{\partial p}\,. \tag{35}$$

When (35) is substituted in (34) we obtain

$$\hat{F}'\psi = \left(F - \left(p(p_0, q_0)\left(\frac{\partial p_0}{\partial p}\right)_q\right)\frac{\partial F}{\partial p_0} - \left(p(p_0, q_0)\left(\frac{\partial q_0}{\partial p}\right)_q\right)\frac{\partial F}{\partial q_0}\right)\psi - i\{F, \psi\}$$

which is of the form (28), and solves the Dirac problem. But we have proved that the most general form of type (28) is

$$\hat{F}'\psi = \left(F - p_0 \frac{\partial F}{\partial p_0} + \{W, F\}\right)\psi - i\{F, \psi\}$$

for some W. It follows that there exists a function $W(p_0, q_0)$ such that

$$-p_0\left(\frac{\partial F}{\partial p_0}\right)_{q_0} + \{W, F\} = -p\left(\frac{\partial F}{\partial p}\right)_q = -p\left(\frac{\partial p_0}{\partial p}\right)_q\left(\frac{\partial F}{\partial p_0}\right)_{q_0} - p\left(\frac{\partial q_0}{\partial p}\right)_q\left(\frac{\partial F}{\partial q_0}\right)_{p_0}$$

[1] We choose units so that $\hbar = 1$.

for all functions F. Clearly we must have

$$-p_0 + \left(\frac{\partial W}{\partial q_0}\right)_{p_0} = -p\left(\frac{\partial p_0}{\partial p}\right)_q \tag{36}$$

$$\left(\frac{\partial W}{\partial p_0}\right)_{q_0} = p\left(\frac{\partial q_0}{\partial p}\right)_q \tag{37}$$

We now show that W can be identified with the Hamilton-Jacobi function for the transformation $(p_0, q_0) \to (p, q)$; for any canonical transformation $(p_0, q_0) \to (p, q)$ that has the property that (q_0, q) form a coordinate set for $\mathfrak{M}$, there exists a function on $\mathfrak{M}$, call it W', which when expressed in terms of (q_0, q) satisfies

$$p_0 = \left(\frac{\partial W'}{\partial q_0}\right)_q, \quad -p = \left(\frac{\partial W'}{\partial q}\right)_{q_0}$$

(see, for example, GOLDSTEIN [21]).

We therefore see that

$$\left(\frac{\partial W'}{\partial q_0}\right)_{p_0} = \left(\frac{\partial W'}{\partial q_0}\right)_q + \left(\frac{\partial W'}{\partial q}\right)_{q_0}\left(\frac{\partial q}{\partial q_0}\right)_{p_0} = p_0 - p\left(\frac{\partial q}{\partial q_0}\right)_{p_0} \tag{38}$$

$$\left(\frac{\partial W'}{\partial p_0}\right)_{q_0} = \left(\frac{\partial W'}{\partial q}\right)_{q_0}\left(\frac{\partial q}{\partial p_0}\right)_{q_0} = -p\left(\frac{\partial q}{\partial p_0}\right)_{q_0} \tag{39}$$

Thus W can be identified with W'. apart from a constant, provided we can prove that

$$\left(\frac{\partial p_0}{\partial p}\right)_q = \left(\frac{\partial q}{\partial q_0}\right)_{p_0} \tag{40}$$

$$\left(\frac{\partial q_0}{\partial p}\right)_q = -\left(\frac{\partial q}{\partial p_0}\right)_{q_0} \tag{41}$$

as is seen by comparing (38) with (36) and (39) with (37).

To prove (40), write

$$dp = \frac{\partial p}{\partial p_0} dp_0 + \frac{\partial p}{\partial q_0} dq_0 \tag{42}$$

$$dq = \frac{\partial q}{\partial p_0} dp_0 + \frac{\partial q}{\partial q_0} dq_0 \,. \tag{43}$$

To find $\left(\frac{\partial p_0}{\partial p}\right)_q$ we put $dq = 0$. So, from (43),

$$dq_0 = -\frac{\partial q}{\partial p_0} \Big/ \frac{\partial q}{\partial q_0} dp_0$$

and from (42)

$$dp = \frac{\partial p}{\partial p_0} dp_0 + \frac{\partial p}{\partial q_0}\left(-\frac{\partial q}{\partial p_0} \Big/ \frac{\partial q}{\partial q_0}\right) dp_0 = \frac{\{q, p\}}{\dfrac{\partial q}{\partial q_0}} dp_0 \,.$$

Therefore $\left(\frac{\partial p_0}{\partial p}\right)_q = \left(\frac{\partial q}{\partial q_0}\right)_{p_0}$, since $\{q, p\} = 1$. Similarly one proves (41). Thus we have proved that on change of coordinates (33) becomes (34) which is

$$\hat{F}'\psi = \left(F - p\frac{\partial F}{\partial p}\right)\psi - i\{F, \psi\} = \left(F - p_0\frac{\partial F}{\partial p_0} + \{W, F\}\right)\psi - i\{F, \psi\}$$

where W is the Hamilton-Jacobi generator of the change of coordinates $(p_0, q_0) \to (p, q)$.

It is easy to see that the different quantizations obtained by making canonical transformations in this way are all unitary equivalent (for a finite number of degrees of freedom). This means the following. Let $\sigma(p_0, q_0) = (p, q)$ be a canonical transformation. Then there exists a unitary operator $U(\sigma)$ on $\mathscr{L}^2(\mathbf{R}^2)$ such that

$$U(\sigma)\,\hat{F}\,U^{-1}(\sigma) = \hat{F}' \quad \text{for all } F$$

with $\hat{F}$ given by (33) and $\hat{F}'$ by (34).

For many purposes it is useful to formulate the canonical quantization procedure in a way that gives the same answer in all coordinates, and not merely equivalent answers.

Let X be a dynamical variable, that is, a function on $\mathfrak{M}$; X will generate a one-parameter group of transformations on $\mathfrak{M}$, given by the classical path $(q(\tau), p(\tau))$ satisfying

$$\frac{dq}{d\tau} = \frac{\partial X}{\partial p}, \quad \frac{dp}{d\tau} = -\frac{\partial X}{\partial q}. \tag{44}$$

We now quantize X according to

$$\hat{X}\psi = \left(X - p\frac{\partial X}{\partial p} + \{W, X\}\right)\psi - i\{X, \psi\}. \tag{45}$$

It is clear that if we choose W such that

$$X - p\frac{\partial X}{\partial p} = -\{W, X\} = \frac{\partial W}{\partial p}\frac{\partial X}{\partial q} - \frac{\partial W}{\partial q}\frac{\partial X}{\partial p} \tag{46}$$

then the quantization of X becomes

$$i\hat{X}\psi = \{X, \psi\}. \tag{47}$$

In this case the "Souriau path" would coincide with the classical path. To find solutions W to (46) given X, remark that both sides are functions of (p, q), and so implicitly they depend on τ. Using (44) we see that (46) becomes

$$X - p\frac{\partial X}{\partial p} = -\frac{dW}{d\tau} \tag{48}$$

so that

$$W = -\int_{\tau_0}^{\tau}\left(X - p\frac{\partial X}{\partial p}\right)d\tau'. \tag{49}$$

The lower limit is chosen at a point where W vanishes, say. The integral is along the classical path, up to the value τ at which the quantization (45) takes place [this means, we are using the coordinates $(p(\tau), q(\tau))$ in (45), abbreviated to (p, q)]. If X is the Hamiltonian, then W is the action integral along the path, i.e. the Lagrangian, which is well-known to give time-displacements in the Halmilton-Jacobi theory. Thus we have rederived the previous result showing how (45) transforms on a change of coordinates from $(p(\tau_0), q(\tau_0))$ (in which $W = 0$) to the coordinates $(p(\tau), q(\tau))$.

In classical mechanics, functions such as W are not dynamical variables; they do not keep the same numerical value when we change coordinates. Thus W depends not only on p and q, but on the two coordinate systems $(p(\tau_0), q(\tau_0))$ and $(p(\tau), q(\tau))$ as well, and expresses the relation between them (in an implicit way). If we keep τ_0 fixed, W is a function of p, q and τ i.e. a function on $\mathfrak{M} \times \mathbf{R}$. But the τ-dependence is of a particularly simple form, namely

$$W(p, q, \tau) = W(p(\tau), q(\tau))$$

for some function W of two variables (we assume τ_0 chosen so that the action vanishes; $\tau_0 = -\infty$ will be chosen in field theory, where the W in the symmetrical form (32), vanishes).

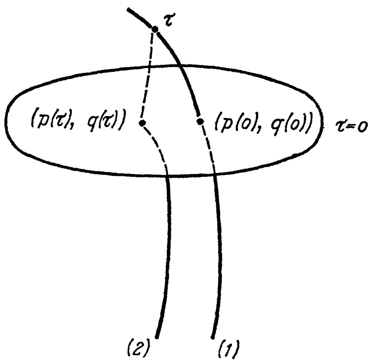

Fig. 1

To see this, consider the function of $p(0)$, $q(0)$

$$W(p(0), q(0)) = \int\limits_{(1)}^{0} \left(X - p\frac{\partial X}{\partial p}\right) d\tau'$$

over the path (1), which ends at $(p(0), q(0))$. The value of the function

$$W(p(0), q(0), \tau) \quad \text{is} \quad \int\limits_{\substack{-\infty \\ (1)}}^{\tau} \left(X - p\frac{\partial X}{\partial p}\right) d\tau'$$

which is equal to $\int\limits_{(2)}^{0} \left(X - p\frac{\partial X}{\partial p}\right) d\tau'$ i.e., the value of the function $W(p(\tau), q(\tau))$. This proves the result. Thus under a change of coordinates $(p, q) \to (p(\tau), q(\tau))$ a transformation function W changes its value according to $W(p, q) \to W(p(\tau), q(\tau))$, i.e. keeps the same functional form in terms of the new variables.

We conclude that equation (32) is form invariant under canonical changes of coordinates if W is taken to transform according to the above rule for transformation functions. Moreover, if W is the action, the quantization is such that the Souriau path coincides with the classical path.

For Eq. (1) Segal has proved [9], [10] that there exist weak limits of $\phi(\mathbf{x}, t)$ (as a limit of t-dependent elements in the space of Cauchy data) as $t \to \pm\infty$; the field converges to solutions of the free equation, which can be used as coordinates to parametrize the manifold of solutions. Thus for a class of $\phi^{\rm in}(\mathbf{x}, t)$, the Cauchy data $(\phi^{\rm in}(\mathbf{x}, 0), \dot\phi^{\rm in}(\mathbf{x}, 0))$ determine a point in $\mathfrak{M}$. Similarly $\phi^{\rm out}(\mathbf{x}, t)$ exists as a weak limit. Segal has also studied [9], [10] the question of the uniqueness of the asymptotic fields. The asymptotic fields are in many ways the most natural coordinates to use. Thus, using (9) to quantize in these coordinates we obtain the following rule for quantizing the smeared field $\phi(f)$.

$$\begin{aligned}\widehat{\phi(f)}\Psi = \Big(\phi(f) &- \frac{1}{2}\int \dot\phi^{\rm in}(\mathbf{x}, 0)\,\frac{\delta\phi(f)}{\delta\dot\phi^{\rm in}(\mathbf{x},0)}\,d^3x - \\ -\frac{1}{2}\int \phi^{\rm in}(\mathbf{x}, 0)\,\frac{\delta\phi(f)}{\delta\phi^{\rm in}(\mathbf{x},0)}\,d^3x\Big)\Psi &- i\int \frac{\delta\phi(f)}{\delta\phi^{\rm in}(\mathbf{x},0)}\,\frac{\delta\Psi}{\delta\dot\phi^{\rm in}(\mathbf{x},0)}\,d^3x + \\ + i\int \frac{\delta\phi(f)}{\delta\dot\phi^{\rm in}(\mathbf{x},0)}\,\frac{\delta\Psi}{\delta\phi^{\rm in}(\mathbf{x},0)}\,d^3x\,. &\end{aligned} \tag{50}$$

This quantization rule has the advantage that the Hamiltonian, and indeed the whole set of generators of the Poincaré group, is quantized by the Koopman rule, that is, these operators generate the classical motion. This is because these dynamical variables are quadratic functions of the in-fields, and so the non-Koopman part of the expression vanishes. We have used the coordinates $(\phi^{\rm in}(\mathbf{x}, 0), \dot\phi^{\rm in}(\mathbf{x}, 0))$ in Eq. (50); the quantization is unchanged if we use $(\phi^{\rm in}(\mathbf{x}, t), \dot\phi^{\rm in}(\mathbf{x}, t))$ for any time t. We let $t \to -\infty$ and then propagate back to $t = 0$ using the same values of the Cauchy data but propagating according to the non-linear equation. By the transformation theory developed above, we can rewrite (50) in terms of the coordinates given by the interacting field at time t. In this case the transformation function is given by

$$S(t) = \int_{-\infty}^{t} dt' \Big\{H - \frac{1}{2}\int \phi(\mathbf{x}, t')\,\frac{\delta H}{\delta\phi(\mathbf{x}, t')}\,d^3x - \frac{1}{2}\int \dot\phi(\mathbf{x}, t')\,\frac{\delta H}{\delta\dot\phi(\mathbf{x}, t')}\,d^3x\Big\} \tag{51}$$

since this form for the action vanishes at $t = -\infty$. For the system given by Eq. (1) the action (51) is

$$S(t) = -\frac{\lambda}{4} \int_{-\infty}^{t} dt' \int d^3x \, \phi^4(\mathrm{x}, t') \,. \tag{52}$$

Segal has shown that for the class of solutions considered by him, $S(t)$ exists and is a smooth function on the manifold.

We may, therefore, rewrite (50) as

$$\begin{aligned} \widehat{\phi(f)}\,\Psi = \Big(\phi(f) - \frac{1}{2}\int \phi(\mathrm{x}, t) \frac{\delta\phi(f)}{\delta\phi(\mathrm{x}, t)}\, d^3x \,- \\ -\frac{1}{2}\int \dot{\phi}(x, t)\frac{\delta\phi(f)}{\delta\dot{\phi}(\mathrm{x}, t)}\, d^3x + \int \frac{\delta S(t)}{\delta\phi(\mathrm{x}, t)} \frac{\delta\phi(f)\, d^3x}{\delta\dot{\phi}(\mathrm{x}, t)} \,- \\ -\int \frac{\delta S(t)}{\delta\dot{\phi}(\mathrm{x}, t)} \frac{\delta\phi(f)}{\delta\phi(\mathrm{x}, t)}\, d^3x\Big)\,\Psi - i\{\phi(f), \Psi\} \,. \end{aligned} \tag{53}$$

Segal's suggestion [11], [12] for the field operator differs from (53) by the omission of the terms involving the action $S(t)$. Because of this, his field operators do not satisfy (7), at least, not as an identity on smooth functionals. The field given by (53) naturally satisfies (7) since (7) is a Lie bracket relation [and (53) solves the Dirac problem]; it will also satisfy local commutativity, relativity and the canonical commutation relations. But it must be emphasized that these relations hold only as relations between transformations of the space of functionals Ψ on $\mathfrak{M}$. Until we put a suitable scalar product on this space (say by a method of functional integration) we cannot assert that $\hat{\phi}(f)$ is a operator on a Hilbert space. We return to this problem later, without solving it however.

4. Quantization of systems with fermions

There is no analogy of Poisson brackets for spinor fields, and so there is no classical Lie algebra to which we can apply the above rules. However, there certainly exists a corresponding c-number theory, defined as the complex-valued solutions ψ of the coupled non-linear partial differential equations appropriate to the problem. For example, for the pseudo-scalar theory of the π^0 interacting with neutrons, the equations have the form

$$(\partial_\mu \gamma_\mu + m)\, \psi(x) = g\, \phi(x)\, \gamma_5 \psi(x) \tag{54}$$

$$(\Box + m^2)\, \phi(x) = g\bar{\psi}(x)\, \gamma_5 \psi(x) \,. \tag{55}$$

In this case one is looking for global smooth solutions with ψ complex and ϕ real; unlike for Eq. (1) the proof that such solutions exist has not yet been given. We shall therefore proceed heuristically. (For the similar equations of electrodynamics, L. Gross has recently proved the existence of local solutions). The idea presented below does not depend on there being a physical interpretation of the c-number function $\psi(x)$ (see the remarks on the difficulties of this in JOST [3]).

We propose to define the classical algebra $\mathfrak{G}$ for the theory to be the set of *gauge-invariant* functionals on the space of c-number solutions. A functional will be said to be gauge invariant if

$$F(\phi, \psi) = F(\phi, e^{i\alpha}\psi)$$

for any real number α. Functionals of this sort, roughly speaking, contain the same number of ψ as ψ^* in each monomial. We may make them into a Lie algebra by defining the Poisson bracket, and then we can proceed as above. For example, for Eq. (54) and (55) the solution is presumably determined by the values of $\phi(\mathbf{x}, 0)$, $\dot{\phi}(\mathbf{x}, 0)$, $\psi(\mathbf{x}, 0)$ and $\bar{\psi}(x, 0)$. The actual independent variables are $\operatorname{Re}\psi$ and $\operatorname{Im}\psi$; ψ and $\bar{\psi} = \psi^* \gamma_0$ may be used formally, since they are linear combinations of them. One may then define

$$\{F, G\} = \int \frac{\delta F}{\delta\phi(\mathbf{x},0)} \frac{\delta G}{\delta\dot{\phi}(\mathbf{x},0)} d^3x - \int \frac{\delta F}{\delta\dot{\phi}(\mathbf{x},0)} \frac{\delta G}{\delta\phi(\mathbf{x},0)} d^3x + \\ + \int \frac{\delta F}{\delta\psi(\mathbf{x},0)} \frac{\delta G}{\delta\bar{\psi}(\mathbf{x},0)} d^3x - \int \frac{\delta F}{\delta\bar{\psi}(\mathbf{x},0)} \frac{\delta G}{\delta\psi(\mathbf{x},0)} d^3x \,. \tag{56}$$

This is gauge invariant if both F and G are. The set of quantized operators thus obtained does not contain any Fermion fields; the approach is therefore best done within the HAAG-ARAKI framework of quantum field theory [5]. While the algebra $\mathfrak{G}$ does not contain all field operators, there is no reason to restrict oneself to observable fields only. Thus in electrodynamics one may quantize any tensor field, including the potentials A_μ, which are not themselves observables. In the realization of a theory with Fermions, the different charge sectors of states [22] will be smooth functionals of the solutions that are respectively gauge invariant, linear in ψ, quadratic in ψ, etc. Each of these spaces would be mapped into itself by the algebra.

According to a recent construction of BORCHERS [23] one might be able to define quasi-local operators carrying the Fermion quantum numbers, from a knowledge of the algebra of observables alone. However, it ought to be possible to construct the Fermion field itself by an extension of the treatment of the present paper.

5. Concluding remarks

The main obstacle to finishing the program outlined here is the problem of finding a suitable method of functional integration; this is also the difficulty in the rather similar program of SEGAL [6]. We now discuss what is meant by suitable functional integral, and the chances of finding one. The meaning of "suitable method of functional integration" depends on the required properties of the field operators and of the theory in general. Let us define the quantitized field by (50), so that that the Poincaré group acts classically on the space of functionals. If one insists that $\hat{\phi}(f)$, as an operator in the eventual Hilbert space, is a WIGHTMAN field, then the scalar product between functionals must satisfy a number of stringent conditions. Certain of the WIGHTMAN postulates, such as the distribution character of $\hat{\phi}(f)$, seem rather unnatural in this formalism. But there must remain a minimum set of conditions to be satisfied, not only for physical reasons, but in order to give a theory which is analytically tractable and not too arbitrary. Since local commutativity will always hold, the determining rôle will be played by the axiom of positive energy. We shall, therefore, require that the scalar product be given by a Poincaré invariant method of functional integration, such that, if Ψ is "square integrable", then so is $\Psi_{a,\Lambda}$. Here, $\Psi_{a,\Lambda}$ is the functional defined by

$$\Psi_{a,\Lambda}(\phi) = \Psi(\phi_{a,\Lambda})$$

where $\phi_{a,\Lambda}(x) = \phi(\Lambda^{-1}(x-a))$. The requirement that the resulting representation of the Poincaré group be continuous puts further conditions on the choice of functional integral. Finally, one would hope that the generator of the time-translations have a spectrum that is bounded below.

In order to get fields in the theory, it is necessary that for a dense set of square-integrable functionals Ψ, the functionals $\hat{\phi}(f)\Psi$ are also square integrable, at least for a class of test-functions f.

These remarks emphasize how difficult it is to find suitable methods of functional integration.

It is not necessary for the chosen subset of square-integrable functionals to be mapped into itself by all dynamical variables, quantized according to (3). In order to get a theory that might legitimately be called a field theory, only the field itself and the Poincaré group, say, need have this property. Thus in the final Hilbert space $\mathscr{H}$ given by square-integrable functionals, we have lost the representation of $\mathfrak{G}$ given by SOURIAU's formula. While the Dirac problem appears to be too ambitious, it turns out to be a very useful and systematic way to find field operators satisfying a non-linear equation such as (7); it is difficult to see how one could have solved (7) without solving first the larger problem posed by Dirac.

It might be thought that our program is too ambitious for another reason, and so unlikely to succeed. For we discuss fields at sharp time, and it would seem from Eq. (7) that there is no necessity for coupling-constant renormalization; there is a general feeling that in a realistic theory, Eq. (7) should be divergent. Now such a situation could quite well happen in the present theory; it is possible that the field operators at sharp time are undefined as operators, since they might not preserve the square-integrability of the functionals when applied to them. In this way the conventional divergences would show up, without, of course, upsetting the finiteness of the theory in terms of the four-dimensional space-time smeared fields. In such a case Eq. (7) itself would have no meaning as an operator equation on Hilbert space, but would still hold on the larger space of smooth functionals. In this sense one could claim to have "solved" Eq. (1).

It might be worth remarking that for Eq. (1) one can show that there exists a Lorentz invariant method of functionals integration; the resulting theory is not likely, however, to have positive energy. This functional integral is obtained as follows.

The manifold of solutions to (1) can be parametrized by the in-field $\phi^{\text{in}}(x)$, and these fields form in a natural way the one-particle representation space $\mathscr{H}_0$ for the Poincaré group. The set of cylinder functions on $\mathscr{H}_0$ is invariant under the action of the Poincaré group; we obtain a space $\mathscr{K}$ by defining the scalar product between cylinder functions on $\mathscr{H}_0$ by means of the Gaussian distribution on $\mathscr{H}_0$. We may define the quantized fields $\hat{\phi}^{\text{in}}$, $\hat{\phi}$ and $\hat{\phi}^{\text{out}}$ on this space directly by equation (50), if we ignore the domain problems of $\hat{\phi}$ and $\hat{\phi}^{\text{out}}$. If we restrict $\mathscr{K}$ to contain only the anti-holomorphic functions, the action of $\hat{\phi}^{\text{in}}$ becomes identical [17] with the Fock representation of the free field, and the energy is bounded below. This Hilbert space is naturally identified with the space $\mathscr{H}^{\text{in}}$ of incoming states.

In defining the interacting field by (50) one meets with a difficulty which is purely algebraic: the field operator $\hat{\phi}(f)$ will take an anti-holomorphic function on $\mathscr{H}_0$ into one not anti-holomorphic, as far as can be seen. Thus in the suggested method of functional integration, the field will not map $\mathscr{H}^{\text{in}}$ into itself; not only will asymptotic completeness be violated, but states created by the interacting field will have energy less than the asymptotic vacuum. In the same way, $\hat{\phi}^{\text{out}}$ will not preserve the anti-holomorphy of the functions, so that this method of functional integration will not work, if we insist that the energy is positive in all states. Whether a suitable method of integration without this drawback exists is an open question.

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