# Dynamical Theory in Curved Spaces. I. A Review of the Classical and Quantum Action Principles*

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## INTRODUCTION

STUDY of the dynamical behavior of quantized physical systems, since the beginning of the quantum theory, has been almost exclusively restricted to systems satisfying either the requirements of nonrelativistic mechanics or, in the case of quantized fields, the requirements of special relativity. This paper is the first of a projected series, to appear in various journals, which will be devoted to extending the quantum theory to the basically broader context of general relativity.

The eventual program envisaged falls naturally into four parts: (1) Study and development of a number of usually neglected aspects of standard quantum mechanics which must be considered when attention is focused on the *nonlinear* features arising from the metric structure of the configuration space of a certain general class of systems. (2) Specialization to those members of this general class in which the specific covariant geometry of a four-dimensional continuum plays the leading role. (3) The carrying out of a reformulation of the "traditional" theory, in which specialized aspects of general relativity become prominently displayed. (4) A study of interacting systems, including those of the Fermi type which possess no classical analogs, in the context of general relativity.

In the following sections a start is made on the first of these four parts. The prototype for the general class of systems to be considered is the system consisting of a nonrelativistic particle moving in a curved space of $n$ dimensions. The extension of standard quantum mechanics to this system is quite straightforward and involves nothing new. However, the notational developments required for the statement of well-known theorems in the context of curved spaces are generally unfamiliar. Therefore it was deemed worthwhile to begin at the beginning, and retrace familiar ground in considerable detail.

The motivation for the general program outlined is, of course, a desire ultimately to attack the problem of the role played by gravitation in the quantum domain. No apology will be made for this motivation, although needless to say, recent experiments have nothing to do with it![1] In the author's opinion it is sufficient that the problem is *there*, like the alpinist's mountain. Beyond that, however, the historical development of physics teaches a suggestive lesson in this connection, namely, that the existence of any fundamental theoretical structure which is far from having been pushed to its logical mathematical conclusions[2] is a situation which may have great potentialities.

The present work follows the traditional path in emphasizing classical-quantum analogies. At the same time an attempt is made to present the material from as modern a viewpoint as possible. In recent years a number of formal mathematical techniques have been developed which have a capacity for coming to grips with various physical problems in a more direct fashion than older methods, and which, owing to the additional insights which they therefore bestow, may eventually transform even the pedagogical approach to the quantum theory. Chief among these techniques are the quantization methods of Feynman[3] and Schwinger[4] and their various extensions, involving functional integration or differentiation and the analysis of the many characteristic Green's functions or "propagation functions" to which they give easy access. Since the problem of the quantum role of gravitation may justly be regarded as one of the most formidable in theoretical physics, it is well to have as many of these new methods available for use as possible. Accordingly, special attention is devoted in the following sections to the classical and quantum action principles, and a study of Feynman quantization in curved spaces is incorporated. The development presents no difficulty, but leads to a slight surprise, a rather curious ambiguity in the definition of the quantum Hamiltonian, involving the invariant curvature.

Extension of Schwinger's theory to curved spaces, on the other hand, is a different matter, and there is some doubt that it can be done at all, at least without extensive modification. Several independent serious efforts in this direction have thus far produced no success,[5]

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[1] The total lack of pertinent experimental information is at once obvious if one recalls that the characteristic length for quantum-gravidynamical processes is $(\hbar G/c^3)^{\frac{1}{2}} \approx 10^{-33}$ cm (where $G$ is the universal gravitation constant) corresponding to energies of the order of $10^{19}$ Bev.

[2] E.g., pre-Lorentzian electrodynamics, or pre-Lambian quantum electrodynamics.

[3] R. P. Feynman, Revs. Modern Phys. **20**, 327 (1948).

[4] J. Schwinger, Phys. Rev. **82**, 914 (1951). No attempt is made to compile a bibliography of the Feynman-Schwinger theory. Among the principal contributors mention may be made of Peierls, Edwards, Salam, Matthews, Källen, Lehmann, and Nambu.

[5] Private communication from P. G. Bergmann, and unpublished work of the author.

although the problem must presently be regarded as still an open one.

Subsequent papers will deal with the important problems posed by the existence of constraints, with systems obeying Fermi statistics in a nonlinear context, and finally with the actual quantization procedure for the gravitational field. An interesting fact will be noted in the course of this development, namely, that whenever a system possesses a classical analog, its quantum theory is in every case essentially completely determined by the corresponding classical theory. This may be regarded as the ultimate extension of Bohr's famous correspondence principle.

## 1. CLASSICAL TRANSFORMATION THEORY

A classical dynamical system is described by means of a set of $2n$ variables $q^i$, $p_i$, $i=1\cdots n$, which, if the system is subject to no constraints, may at a given initial instant be independently specified. The $q^i$ are commonly known as *coordinates* and the $p_i$ as *momenta*. The fact that $n$ may be nondenumerably infinite for many systems of primary interest is of no importance in the present discussion. The simplicity of the formal mathematics for the finite case will be retained throughout, it being tacitly assumed (as is in fact the case) that the limiting procedures implied in the passage to continuum cases involve no difficulties of principle.

An experimental measurement performed on a physical system generally gives information about the value of some function(al) $F$ of the $q$'s and $p$'s. $F$ is known as a physical *observable*. In the classical theory any function(al) of the $q$'s and $p$'s is, in principle, an observable.

Of fundamental importance in the development of the dynamical theory is the *Poisson bracket* of two observables $F$ and $G$, which is defined by

$$(F,G) \equiv \frac{\partial F}{\partial q^i}\frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial G}{\partial q^i}. \qquad (1.1)$$

In this paper, a summation is to be understood over repeated indexes unless the contrary is explicitly stated. For many purposes it is convenient to introduce a slightly more compact notation through the replacements

$$x_i{}^1 \equiv q^i, \quad x_i{}^2 \equiv p_i. \qquad (1.2)$$

Equation (1.1) may then be rewritten in the form

$$(F,G) \equiv \epsilon_{\alpha\beta}\frac{\partial F}{\partial x_i{}^\alpha}\frac{\partial G}{\partial x_i{}^\beta}, \qquad (1.3)$$

where $\epsilon_{\alpha b}$ is the two-dimensional antisymmetric permutation symbol, the indexes $\alpha$ and $\beta$ ranging over the values 1, 2.

The notation of (1.2) and (1.3) emphasizes the symmetry between coordinates and momenta which is characteristic of both classical and quantum transformation theory and which has its quantum expression in the

wave-particle dualism. This symmetry does not, however, persist in detail in the dynamical theory of actual physical systems.[6] This fact has been anticipated here by the difference in the position of the index on the $q$'s and $p$'s.

From (1.1) or (1.3) the well-known corollaries follow immediately

$$(F_1,F_2) = -(F_2,F_1), \qquad (1.4)$$

$$(F,f(F_1,F_2\cdots))$$
$$= (F,F_1)\partial f/\partial F_1 + (F,F_2)\partial f/\partial F_2 + \cdots. \qquad (1.5)$$

Also the Poisson-Jacobi identity

$$(F_1,(F_2,F_3)) + (F_2,(F_3,F_1)) + (F_3,(F_1,F_2)) = 0, \qquad (1.6)$$

may be obtained with the aid of the three-dimensional permutation symbol $\epsilon_{abc}$ in terms of which the left side of (1.6) may be written

$$\tfrac{1}{2}\epsilon_{abc}(F_a,(F_b,F_c)) = \epsilon_{abc}\epsilon_{\alpha\beta}\epsilon_{\gamma\delta}\frac{\partial F_a}{\partial x_i{}^\alpha}\frac{\partial F_b}{\partial x_j{}^\gamma}\frac{\partial^2 F_c}{\partial x_i{}^\beta \partial x_j{}^\delta}.$$

The quantity multiplying $\epsilon_{abc}$ in the latter expression is symmetric in $a$ and $b$, and hence the whole expression vanishes.

Consider a transformation in the description of a dynamical system, from the variables $q^i$, $p_i$ (or $x_i{}^\alpha$) to a set of variables $\xi_\mu$, $\mu=1\cdots 2n$. Consider the $2n$-dimensional antisymmetric matrix formed by taking the Poisson brackets of all possible pairs $\xi_\mu$, $\xi_\nu$. Using the notation of (1.3) it is not difficult to show that the determinant of this matrix is given by

$$|(\xi_\mu,\xi_\nu)| = [\partial(x)/\partial(\xi)]^2. \qquad (1.7)$$

Evidently, if the Jacobian $\partial(x)/\partial(\xi)$ of the transformation $x_i{}^\alpha \to \xi_\mu$ is nonvanishing the matrix $(\xi_\mu,\xi_\nu)$ has an inverse. This inverse defines the so-called *Lagrange bracket*[7] $[\![\xi_\mu,\xi_\nu]\!]$, satisfying

$$[\![\xi_\mu,\xi_\sigma]\!](\xi_\nu,\xi_\sigma) = \delta_{\mu\nu}. \qquad (1.8)$$

Since

$$\epsilon_{\alpha\gamma}\epsilon_{\beta\gamma} = \delta_{\alpha\beta}, \qquad (1.9)$$

the Lagrange bracket is given explicitly by

$$[\![\xi_\mu,\xi_\nu]\!] \equiv \epsilon_{\alpha\beta}\frac{\partial x_i{}^\alpha}{\partial\xi_\mu}\frac{\partial x_i{}^\beta}{\partial\xi_\nu} \equiv -[\![\xi_\nu,\xi_\mu]\!]. \qquad (1.10)$$

Out of the set of all possible transformations $q^i$, $p_i \to \xi_\mu$ classical dynamics focuses attention on certain special ones known as *canonical transformations*. The set of all canonical transformations may be defined as

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[6] Notwithstanding the fact that the symmetry idea has been sufficiently impressive to have been invoked on at least two occasions as a rigorous dynamical principle: M. Born, Proc. Roy. Soc. (London) A165, 291 (1938); H. Yukawa, Phys. Rev. 77, 219 (1950).

[7] Whittaker [*Analytical Dynamics* (Cambridge University Press, New York, 1937), p. 298] uses the symbols ( ) and [ ] for the Poisson and Lagrange brackets, respectively. The symbol [ ] is, however, here reserved for the commutator bracket used in the quantum theory.

the most general set of transformations $q^i$, $p_i \rightarrow \bar{q}^i$, $\bar{p}_i$ (or $x_i^\alpha \rightarrow \bar{x}_i^\alpha$) such that

(i) there exists an essentially unique (up to trivial modifications) differential form of the type

$$A\bar{p}_i d\bar{q}^i + B\bar{q}^i d\bar{p}_i + Cp_i dq^i + Dq^i dp_i,$$

which is an exact differential for all members of the set.[8]

(ii) The members of the set form a group.

It must be specified that the coefficients $A$, $B$, $C$, $D$ are independent of the $p$'s and $q$'s, and trivial cases may be excluded by imposing the conditions

$$A \neq B, \quad C \neq D. \tag{1.11}$$

Furthermore, the trivial exact differential

$$\tfrac{1}{2}(A+B)(\bar{p}_i d\bar{q}^i + \bar{q}^i d\bar{p}_i) + \tfrac{1}{2}(C+D)(p_i dq^i + q^i dp_i),$$

may be subtracted from the original form, and the result divided by $\tfrac{1}{2}(A-B)$ to obtain a canonical form

$$\bar{p}_i d\bar{q}^i - \bar{q}^i d\bar{p}_i + \zeta(p_i dq^i - q^i dp_i), \tag{1.12}$$

where $\zeta = (C-D)/(A-B)$. In order that a second transformation $\bar{q}^i$, $\bar{p}_i \rightarrow \tilde{q}^i$, $\tilde{p}_i$ be canonical the expression

$$\tilde{p}_i d\tilde{q}^i - \tilde{q}^i d\tilde{p}_i + \zeta(\bar{p}_i d\bar{q}^i - \bar{q}^i d\bar{p}_i), \tag{1.13}$$

must also be an exact differential. The group property of canonical transformations may then be applied to the result of subtracting $\zeta$ times (1.12) from (1.13), leading to the condition $\zeta^2 = -\zeta$, or

$$\zeta = -1. \tag{1.14}$$

Therefore, the set of all canonical transformations may be characterized by the statement

$$\begin{aligned}\bar{p}_i d\bar{q}^i - \bar{q}^i d\bar{p}_i - p_i dq^i + q^i dp_i \\ = \epsilon_{\alpha\beta}(x_i^\alpha dx_i^\beta - \bar{x}_i^\alpha d\bar{x}_i^\beta) = dV, \quad (1.15)\end{aligned}$$

for some $V$.

An explicit form for $V$ may depend on any or all of the $q^i$, $p_i$, $\bar{q}^i$, $\bar{p}_i$. However, if $V$ is regarded as a function of the $\bar{q}^i$, $\bar{p}_i$ (or $\bar{x}_i^\alpha$) alone then evidently

$$\frac{\partial V}{\partial \bar{x}_j^\beta} = \epsilon_{\gamma\delta}x_k^\gamma \frac{\partial x_k^\delta}{\partial \bar{x}_j^\beta} - \epsilon_{\alpha\beta}\bar{x}_j^\alpha, \tag{1.16}$$

$$\frac{\partial^2 V}{\partial \bar{x}_i^\alpha \partial \bar{x}_j^\beta} = [\![\bar{x}_i^\alpha, \bar{x}_j^\beta]\!] - \epsilon_{\alpha\beta}\delta_{ij} + \epsilon_{\gamma\delta}x_k^\gamma \frac{\partial^2 x_k^\delta}{\partial \bar{x}_i^\alpha \partial \bar{x}_j^\beta}. \tag{1.17}$$

The expression on the right of (1.17) can be symmetric under interchange of the indexes $i$, $\alpha$ with the indexes $j$, $\beta$ if and only if

$$[\![\bar{x}_i^\alpha, \bar{x}_j^\beta]\!] = \epsilon_{\alpha\beta}\delta_{ij}, \tag{1.18}$$

and hence

$$(\bar{x}_i^\alpha, \bar{x}_j^\beta) = \epsilon_{\alpha\beta}\delta_{ij}. \tag{1.19}$$

Equation (1.18) or (1.19) may be used in place of (1.15) as an equally valid characterization of a canonical transformation.

The importance of canonical transformations lies in the existence of their well-known invariants.[9] For example, the Poisson bracket of two observables $F$ and $G$ remains unchanged if in (1.1) the $q^i$, $p_i$ are replaced by $\bar{q}^i$, $\bar{p}_i$. This is readily shown with the aid of (1.19):

$$(F,G) \equiv \epsilon_{\alpha\beta}\frac{\partial F}{\partial x_i^\alpha}\frac{\partial G}{\partial x_i^\beta} = \epsilon_{\alpha\beta}\frac{\partial \bar{x}_j^\gamma}{\partial x_i^\alpha}\frac{\partial \bar{x}_k^\delta}{\partial x_i^\beta}\frac{\partial F}{\partial \bar{x}_j^\gamma}\frac{\partial G}{\partial \bar{x}_k^\delta}$$

$$= (\bar{x}_j^\gamma, \bar{x}_k^\delta)\frac{\partial F}{\partial \bar{x}_j^\gamma}\frac{\partial G}{\partial \bar{x}_k^\delta} = \overline{(F,G)}. \tag{1.20}$$

Lagrange brackets remain similarly invariant. For many purposes, therefore, the $q^i$, $p_i$ may be replaced by the $\bar{q}^i$, $\bar{p}_i$ as equally valid *canonical* variables.

The explicit construction of canonical transformations is conveniently carried out with the aid of *generators*. Four standard types of generators are commonly considered, which may be denoted by $S_{\pm\pm}$, and which are related to the $V$ of (1.15) by

$$S_{\pm\pm} = \tfrac{1}{2}(V \pm \bar{q}^i \bar{p}_i \pm q^i p_i). \tag{1.21}$$

Computation of $dS_{\pm\pm}$ with the aid of (1.15) shows that the solution of a set of simultaneous equations of any one of the following four types,

$$\bar{p}_i = \partial S_{++}/\partial \bar{q}^i, \qquad q^i = \partial S_{++}/\partial p_i, \tag{1.22a}$$

$$\bar{p}_i = \partial S_{+-}/\partial \bar{q}^i, \qquad p_i = -\partial S_{+-}/\partial q^i, \tag{1.22b}$$

$$\bar{q}^i = -\partial S_{-+}/\partial \bar{p}_i, \quad q^i = \partial S_{-+}/\partial p_i, \tag{1.22c}$$

$$\bar{q}^i = -\partial S_{--}/\partial \bar{p}_i, \quad p_i = -\partial S_{--}/\partial q^i, \tag{1.22d}$$

yields a canonical transformation.[10] Here $S_{++}$ is an arbitrary function of the $p_i$ and $\bar{q}^i$ alone, $S_{+-}$ of the $q^i$ and $\bar{q}^i$ alone, $S_{-+}$ of the $p_i$ and $\bar{p}_i$ alone, and $S_{--}$ of the $q^i$ and $\bar{p}_i$ alone.

Three elementary but important examples of canonical transformations may be obtained immediately with the aid of (1.22a):

(i) *The identity transformation:*

$$S_{++} = p_i \bar{q}^i, \quad \bar{q}^i = q^i, \quad \bar{p}_i = p_i. \tag{1.23}$$

(ii) *"Phase" transformations:*

$$S_{++} = p_i \bar{q}^i + \Phi(\bar{q}), \quad \bar{q}^i = q^i, \quad \bar{p}_i = p_i + \partial \Phi/\partial q^i. \tag{1.24}$$

(iii) *Point transformations:*

$$S_{++} = p_i q^i(\bar{q}), \quad \bar{q}^i = \bar{q}^i(q), \quad \bar{p}_i = p_j(\partial q^j/\partial \bar{q}^i). \tag{1.25}$$

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[8] Here the $d\bar{q}^i$, $d\bar{p}_i$ are to be expressed in terms of the $dq^i$, $dp_i$ or vice versa.

[9] Using (1.18) it is not hard to show that integrals of the form $\int dq^{i_1} dp_{i_1} \cdots dq^{i_m} dp_{i_m}$, $m = 1 \cdots n$, the summation being carried out in such a way that the indexes $i_1 \cdots i_m$ are all different, are canonically invariant. The case $m = n$ yields the canonical invariance of the volume element in phase space, or the alternative fact that the Jacobian of a canonical transformation is equal to $+1$.

[10] The most general canonical transformation can be obtained through a combination of these four types.

Of special importance in the development of the dynamical theory to follow are the *infinitesimal* canonical transformations:

$$\bar{q}^i = q^i + \delta q^i, \quad \bar{p}_i = p_i + \delta p_i, \quad \text{or} \quad \bar{x}_i^\alpha = x_i^\alpha + \delta x_i^\alpha. \quad (1.26)$$

The function $V$ of (1.15) must in this case be an infinitesimal $v$ satisfying

$$dv = -\epsilon_{\alpha\beta}(\delta x_i^\alpha dx_i^\beta + x_i^\alpha d\delta x_i^\beta). \quad (1.27)$$

An *infinitesimal generator* for the transformation is given by

$$s = \tfrac{1}{2}(v + \epsilon_{\alpha\beta}x_i^\alpha \delta x_i^\beta), \quad (1.28)$$

satisfying

$$ds = \epsilon_{\alpha\beta}dx_i^\alpha \delta x_i^\beta, \quad (1.29)$$

so that

$$\partial s/\partial x_i^\alpha = \epsilon_{\alpha\beta}\delta x_i^\beta, \quad \text{or} \quad \delta x_i^\alpha = -\epsilon_{\alpha\beta}\partial s/\partial x_i^\beta, \quad (1.30a)$$

$s$ being expressed as a function of the $x_i^\alpha$ alone. In terms of $q^i$, $p_i$ (1.30a) becomes

$$\delta q^i = -\partial s/\partial p_i, \quad \delta p_i = \partial s/\partial q^i, \quad (1.30b)$$

$s=0$ gives the identity transformation; an infinitesimal phase transformation is given by $s = \varphi(q)$, where $\varphi$ is an infinitesimal function of the coordinates; and an infinitesimal point transformation is given by

$$s = p_i \lambda^i(q), \quad \bar{q}^i = q^i - \lambda^i, \quad \bar{p}_i = p_i + p_j \partial \lambda^j/\partial q^i, \quad (1.31)$$

where the $\lambda^i$ are infinitesimal.

If $F$ is a function(al) of the $q^i$, $p_i$ with fixed functional form, then under the transformation (1.30) its value suffers a change of amount

$$\delta F = (\partial F/\partial x_i^\alpha)\delta x_i^\alpha = -(F,s). \quad (1.32)$$

If, on the other hand, $F$ is regarded as a fixed physical magnitude whose functional dependence on the canonical variables changes under (1.30), the amount of this change may be defined as

$$\bar{\delta}F(q,p) = \bar{F}(q,p) - F(q,p), \quad (1.33)$$

where

$$\bar{F}(\bar{q},\bar{p}) = F(q,p). \quad (1.34)$$

Evidently

$$\bar{\delta}F = -\delta\bar{F} = -\delta F = (F,s), \quad (1.35)$$

correct to the first infinitesimal order.

This last result may be used to rederive the canonical invariance of Poisson brackets under infinitesimal transformations. One writes

$$(F,G) = (\bar{F}(\bar{q},\bar{p}), \bar{G}(\bar{q},\bar{p}))$$
$$= (F(\bar{q},\bar{p}) + \bar{\delta}F(\bar{q},\bar{p}), G(\bar{q},\bar{p}) + \bar{\delta}G(\bar{q},\bar{p}))$$
$$= (F,G) + \delta(F,G) + (F,\bar{\delta}G) + (\bar{\delta}F,G)$$
$$= (F,G) + (s,(F,G)) + (F,(G,s)) + (G,(s,F)),$$

which leads to (1.20) in virtue of the Poisson-Jacobi identity (1.6).

Consider now a finite canonical transformation from a set of variables $x_i^\alpha(1)$ to a second set $x_i^\alpha(2)$. From

(1.15) we have

$$\epsilon_{\alpha\beta}[x_i^\alpha(1)dx_i^\beta(1) - x_i^\alpha(2)dx_i^\beta(2)] = dV, \quad (1.36)$$

where $V$ is some function of the $x_i^\alpha(1)$ and $x_i^\alpha(2)$. Suppose the variables $x_i^\alpha(1)$ and $x_i^\alpha(2)$ are subjected to independent infinitesimal canonical transformations:

$$\bar{x}_i^\alpha(1) = x_i^\alpha(1) + \delta x_i^\alpha(1),$$
$$\delta x_i^\alpha(1) = -\epsilon_{\alpha\beta}\partial s(1)/\partial x_i^\beta(1), \quad (1.37)$$
$$\bar{x}_i^\alpha(2) = x_i^\alpha(2) + \delta x_i^\alpha(2),$$
$$\delta x_i^\alpha(2) = -\epsilon_{\alpha\beta}\partial s(2)/\partial x_i^\beta(2). \quad (1.38)$$

Then there must exist some new function $\bar{V}$ which differs infinitesimally from $V$, such that

$$d\bar{V} = \epsilon_{\alpha\beta}[\bar{x}_i^\alpha(1)d\bar{x}_i^\beta(1) - \bar{x}_i^\alpha(2)d\bar{x}_i^\beta(2)]$$
$$= dV + \epsilon_{\alpha\beta}[\delta x_i^\alpha(1)dx_i^\beta(1) + x_i^\alpha(1)d\delta x_i^\beta(1)$$
$$\quad - \delta x_i^\alpha(2)dx_i^\beta(2) - x_i^\alpha(2)d\delta x_i^\beta(2)]$$
$$= dV + d\{2[s(2) - s(1)]$$
$$\quad + \epsilon_{\alpha\beta}[x_i^\alpha(1)\delta x_i^\beta(1) - x_i^\alpha(2)\delta x_i^\beta(2)]\}. \quad (1.39)$$

Evidently

$$\bar{V} = V + \delta V + \bar{\delta}V, \quad (1.40)$$

where

$$\delta V = \epsilon_{\alpha\beta}[x_i^\alpha(1)\delta x_i^\beta(1) - x_i^\alpha(2)\delta x_i^\beta(2)], \quad (1.41)$$

$$\bar{\delta}V = 2[s(2) - s(1)]. \quad (1.42)$$

The infinitesimal $\bar{\delta}V$ represents a change in the functional *form* of $V$ which is required to characterize the new canonical transformation $\bar{x}_i^\alpha(1) \to \bar{x}_i^\alpha(2)$, whereas $\delta V$ simply represents the change in the value of the original function due to the changes $\delta x_i^\alpha(1)$, $\delta x_i^\alpha(2)$ in the values of the variables.

If the canonical transformation $x_i^\alpha(1) \to x_i^\alpha(2)$ is described by means of one of the generators $S_{\pm\pm}$, then it follows from (1.21) and (1.42) that

$$\bar{\delta}S_{\pm\pm} = s(2) - s(1), \quad (1.43)$$

in which $s(1)$ and $s(2)$ are to be re-expressed in terms of the variables suitable to the generator in question. We therefore have

*Theorem:*

*The variation in the functional form of the generator of a finite canonical transformation, due to independent infinitesimal canonical transformations of its arguments, is equal to the difference of the independent infinitesimal generators.*

## 2. THE CLASSICAL ACTION PRINCIPLE

The "trajectory" of a physical system is described by a set of functions $q^i(t)$, $i=1\cdots n$, which determine the configuration of the system at any time $t$. Classical dynamical theory may be based on the following

*Dynamical postulate:*

*The class of all trajectories $q(t)$ of a physical system is determined by the unfolding-in-time of a canonical transformation.*

This implies the existence, in addition to the "coordinates" $q^i(t)$, of a set of momenta $p_i(t)$ which depend on the trajectory, or which, alternatively, may help to specify the trajectory.

The infinitesimal generator of the canonical transformation $q^i(t)$, $p_i(t) \rightarrow q^i(t+\delta t)$, $p_i(t+\delta t)$, where $\delta t$ is an arbitrary infinitesimal "displacement" in time, will have the general form[11]

$$s = -H(q(t),p(t),t)\delta t, \qquad (2.1)$$

where $H$ is some explicit function of the coordinates and momenta, and possibly also of the time. $H$ is known as the *Hamiltonian function(al)*, or, simply, the *Hamiltonian*, and its exact form depends on the system in question. Equations (1.30b) together with the relations $\delta q^i = \dot{q}^i \delta t$, $\delta p_i = \dot{p}_i \delta t$ lead immediately to the familiar Hamiltonian equations for the trajectory

$$\dot{q}^i = \partial H/\partial p_i, \quad \dot{p}_i = -\partial H/\partial q^i, \qquad (2.2)$$

the dot denoting the total time derivative. From (2.2) it follows that the time rate of change of any physical observable $F$ is given by

$$\dot{F} = (F,H) + \partial F/\partial t \qquad (2.3)$$

[see (1.32)], where the partial derivative $\partial/\partial t$ is taken with respect to any explicit dependence on $t$ which $F$ may have. Since the Poisson bracket is canonically invariant it may be taken with respect to the canonical variables appropriate to the time in question as well as with respect to any other canonical variables. If $F$ and $G$ are any two physical observables the time rate of change of their Poisson bracket is given by

$$d(F,G)/dt = (\dot{F},G) + (F,\dot{G}), \qquad (2.4)$$

which follows from (2.3) together with the Poisson-Jacobi identity (1.6).

The finite canonical transformation which relates the coordinates and momenta at two different times, $t'$ and $t''$, may generally be described by one or more of the four types of generators considered in (1.22). In the present context these equations become

$$p_i(t'') = \partial S_{++}/\partial q^i(t''), \qquad q^i(t') = \partial S_{++}/\partial p_i(t'), \qquad (2.5a)$$

$$p_i(t'') = \partial S_{+-}/\partial q^i(t''), \qquad p_i(t') = -\partial S_{+-}/\partial q^i(t'), \qquad (2.5b)$$

$$q^i(t'') = -\partial S_{-+}/\partial p_i(t''), \qquad q^i(t') = \partial S_{-+}/\partial p_i(t'), \qquad (2.5c)$$

$$q^i(t'') = -\partial S_{--}/\partial p_i(t''), \qquad p_i(t') = -\partial S_{--}/\partial q^i(t'). \qquad (2.5d)$$

Very often we wish to single out a particular value of one of the canonical variables. This is done by affixing one or more primes to the variable in question. The value thus indicated will be *independent* of the particular value of the time involved. Thus,

$$q'^i(t) = q'^i, \quad p'_i(t) = p'_i, \quad \text{independent of } t. \qquad (2.6)$$

To avoid confusion in application of this convention,

the following modification in notation will be introduced:

$$S_{++}(q''(t'') \,|\, p'(t')) = S(q'',t''\,|\,p',t'), \qquad (2.7a)$$

$$S_{+-}(q''(t'') \,|\, q'(t')) = S(q'',t''\,|\,q',t'), \qquad (2.7b)$$

$$S_{-+}(p''(t'') \,|\, p'(t')) = S(p'',t''\,|\,p',t'), \qquad (2.7c)$$

$$S_{--}(p''(t'') \,|\, q'(t')) = S(p'',t''\,|\,q',t'). \qquad (2.7d)$$

That is, the values of the canonical variables and the values of the time will be separately specified in the generating functions. On the other hand, the $+$ and $-$ signs will be dropped, as indicated, since the arguments themselves are sufficient to indicate which generator is meant.

The finite generators must be related in some way to the Hamiltonian which generates the infinitesimal displacements in time. This relation is readily determined with the aid of the theorem of the preceding section, (1.43). For definiteness, consider the function $S(q'',t''\,|\,p',t')$. Let $\delta q''^i$, $\delta t''$, $\delta p'_i$, $\delta t'$ be arbitrary infinitesimal variations in its arguments. The variations $\delta t''$, $\delta t'$ will give rise to a change in the *form* of this generator, considered as a function of the $q''^i$, $p'_i$. From (1.43) and (2.1), the amount of this change is $s'' - s' = -H''\delta t'' + H'\delta t'$ where $H'$ and $H''$ are the values of the Hamiltonian at the times $t'$ and $t''$, respectively, for the particular trajectory specified by the arguments $q''$, $t''$, $p'$, $t'$. The variations $\delta q''^i$, $\delta p'_i$, on the other hand, give rise to a change in *value*, which may be computed with the aid of (2.5a). The total variation in the generator is

$$\delta S(q'',t''\,|\,p',t') = p''_i \delta q''^i - H''\delta t'' + q'^i \delta p'_i + H'\delta t', \qquad (2.8a)$$

where $p''_i = p_i(t'')$, $q'^i = q^i(t')$ for the trajectory in question. Similarly,

$$\delta S(q'',t''\,|\,q',t') = p''_i \delta q''^i - H''\delta t'' - p'_i \delta q'^i + H'\delta t', \qquad (2.8b)$$

$$\delta S(p'',t''\,|\,p',t') = -q''^i \delta p''_i - H''\delta t'' + q'^i \delta p'_i + H'\delta t', \qquad (2.8c)$$

$$\delta S(p'',t''\,|\,q',t') = -q''^i \delta p''_i - H''\delta t'' - p'_i \delta q'^i + H'\delta t'. \qquad (2.8d)$$

By expressing all the quantities on the right of (2.8) in terms of the arguments appearing on the left, one is led to the *Hamilton-Jacobi equations* for the various generators. These are, respectively,

$$\left.\begin{array}{l} \partial S/\partial t'' + H(q'',\partial S/\partial q'',t'') = 0 \\ -\partial S/\partial t' + H(\partial S/\partial p',p',t') = 0 \end{array}\right\} \qquad (2.9a)$$

$$\left.\begin{array}{l} \partial S/\partial t'' + H(q'',\partial S/\partial q'',t'') = 0 \\ -\partial S/\partial t' + H(q', -\partial S/\partial q', t') = 0 \end{array}\right\} \qquad (2.9b)$$

$$\left.\begin{array}{l} \partial S/\partial t'' + H(-\partial S/\partial p'', p'', t'') = 0 \\ -\partial S/\partial t' + H(\partial S/\partial p',p',t') = 0 \end{array}\right\} \qquad (2.9c)$$

$$\left.\begin{array}{l} \partial S/\partial t'' + H(-\partial S/\partial p'', p'', t'') = 0 \\ -\partial S/\partial t' + H(q', -\partial S/\partial q', t') = 0 \end{array}\right\}. \qquad (2.9d)$$

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[11] The minus sign is arbitrary and is chosen to correspond to convention.

In the integration of the Hamiltonian equations (2.2) a given trajectory is generally determined by specifying the $q^i$ and $p_i$ at a given "initial" time. Use of the generating functions, on the other hand, implies a different determination of the trajectory, namely, by specifying either the coordinates *or* the momenta (not both) at two different times. Actually, such a specification is not always possible. For example, if a representation is chosen (as is customary) in which the $q^i$ are physical coordinates, the function $S(p'',t''|p',t')$ may not exist (e.g., in the case of the free particle). On the other hand, the function $S(q'',t''|q',t')$ may be multivalued (as in the case of the particle in a box) reflecting the fact that there may be more than one trajectory (the reflected trajectories) between the space-time points $q'$, $t'$ and $q''$, $t''$.

The function $S(q'',t''|q',t')$ is of special importance in the developments to follow, and is known as the *classical action*. We now study this function in greater detail, ignoring for the time being the possibility of its being multivalued. Let us denote by

$$q^i = (q'',t''|q^i(t)|q',t'),\qquad (2.10)$$

the trajectory determined by the points $q'$, $t'$ and $q''$, $t''$. The explicit form of the right-hand side of (2.10) may be obtained by breaking into the trajectory at time $t$ and solving the set of simultaneous equations

$$-\partial S(q'',t''|q,t)/\partial q^i = p_i(t) = \partial S(q,t|q',t')/\partial q^i. \qquad (2.11)$$

The action $S$ is so far uniquely determined only up to an arbitrary constant. In virtue of (2.11) and the Hamilton-Jacobi equations (2.9b), this constant may be so adjusted that for all $q''$, $q$, $q'$, $t''$, $t$, $t'$,

$$S(q'',t''|q',t') = -S(q',t'|q'',t''), \qquad (2.12)$$

and

$$S(q'',t''|q',t') = [S(q'',t''|q,t)+S(q,t|q',t')]_{q=q_{\text{ext}}}, \qquad (2.13)$$

the instruction "$q=q_{\text{ext}}$" indicating that the quantity in the brackets is to be made an extremal with respect to the $q^i$. The extremal values are given precisely by (2.10).

By breaking the trajectory into infinitely many pieces we see that the action may be regarded as formed in the following way:

$$S(q'',t''|q',t') = \{S[q]_{q',t'}{}^{q'',t''}\}_{q=(q'',t''|q(t)|q',t')}, \qquad (2.14)$$

where $S[q]_{q',t'}{}^{q'',t''}$ is a functional of an arbitrary trajectory $q$ between the points $q'$, $t'$ and $q''$, $t''$, satisfying the variational equation

$$\{\delta S[q]_{q',t'}{}^{q'',t''}/\delta q\}_{q=(q'',t''|q(t)|q',t')} = 0, \qquad (2.15)$$

and the combination laws

$$S[q]_{q',t'}{}^{q'',t''} = S[q]_{q(t),t}{}^{q'',t''} + S[q]_{q',t'}{}^{q(t),t}, \qquad (2.16)$$

$$S[q]_{q',t'}{}^{q'',t''} = -S[q]_{q'',t''}{}^{q',t'}. \qquad (2.17)$$

Equations (2.16) and (2.17) imply that $S[q]$ may be expressed in the form

$$S[q]_{q',t'}{}^{q'',t''} = \int_{q',t'}^{q'',t''} L(q,\dot{q},t)dt. \qquad (2.18)$$

$L$ is a function(al) of the $q^i$ and their time derivatives (and also possibly of the time), known as the *Lagrangian* of the system in question.

When $S[q]$ is expressed in the form (2.18), the variational equation (2.15) is known as the *principle of stationary action*. Performing the indicated variation, with the restrictions $q^i(t')=q'^i$, $q^i(t'')=q''^i$, $\delta q^i(t')=0$, $\delta q^i(t'')=0$, and making an integration by parts, one obtains the familiar Lagrangian "equations of motion" for the trajectory

$$0 = \frac{\partial L}{\partial q^i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i}. \qquad (2.19)$$

Equations (2.19) are of the second order in contrast to the Hamiltonian equations (2.2) which are of the first order.

The relation between the Lagrangian and Hamiltonian functions may be determined with the aid of (2.8b), (2.14), and (2.19). Denote by $\delta q^i(t)$ the variation in a given trajectory produced by variations $\delta q'^i$, $\delta t'$, $\delta q''^i$, $\delta t''$ in its end points. Then, with an obvious notation,

$$\delta q^i(t') = \delta q'^i - \dot{q}'^i\delta t', \qquad \delta q^i(t'') = \delta q''^i - \dot{q}''^i\delta t'', \qquad (2.20)$$

and

$$\delta S(q'',t''|q',t')$$

$$= \delta\left[\int_{t'}^{t''} L dt\right]_{q=(q'',t''|q(t)|q',t')}$$

$$= L''\delta t'' - L'\delta t'$$

$$+ \left[\int_{t'}^{t''} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\delta q^i\right)dt\right]_{q=(q'',t''|q(t)|q',t')}$$

$$= \left(\frac{\partial L}{\partial \dot{q}^i}\right)'' \delta q''^i - \left[\left(\frac{\partial L}{\partial \dot{q}^i}\right)'' \dot{q}''^i - L''\right]\delta t''$$

$$- \left(\frac{\partial L}{\partial \dot{q}^i}\right)' \delta q'^i + \left[\left(\frac{\partial L}{\partial \dot{q}^i}\right)' \dot{q}'^i - L'\right]\delta t'. \qquad (2.21)$$

Comparison of (2.8b) and (2.21) shows that

$$p_i = \partial L/\partial \dot{q}^i, \qquad (2.22)$$

$$H = p_i\dot{q}^i - L. \qquad (2.23)$$

A few tacit assumptions have been made. Firstly, it has been assumed that the Hamiltonian function, and hence the Lagrangian and action functions, are unique for a given system. Actually, a slight lack of uniqueness in these functions is allowed. The physics of a given

system is entirely contained in the Lagrange equations (2.19), and from their variational manner of derivation it is evident that they are unchanged if the Lagrangian is replaced by

$$\bar{L} = L + d\Phi/dt, \tag{2.24}$$

where $\Phi$ is an arbitrary function of the $q^i$ and $t$. This replacement produces a change in the momenta, given by

$$\bar{p}_i = p_i + \partial\Phi/\partial q^i, \tag{2.25}$$

which is simply a phase transformation [(1.24)]. The corresponding transformation of the action is given by

$$\bar{S}[q]_{q', \, t'}^{q'', t''} = S[q]_{q', \, t'}^{q'', t''} + \Phi(q'', t'') - \Phi(q', t'), \tag{2.26}$$

$$\bar{S}(q'', t'' \,|\, q', t') = S(q'', t'' \,|\, q', t') + \Phi(q'', t'') - \Phi(q', t'), \tag{2.27}$$

which leaves the combination laws (2.16, 2.17) invariant. Phase transformations will be employed on several occasions in the future.

Secondly, the assumption that the generating function $S(q'', t'' \,|\, q', t')$ exists at all (at least in some canonical representation) is equivalent to insisting that the first of the Hamiltonian equations (2.2) be solvable for the $p_i$ in terms of the $q^i$, $\dot{q}^i$ (and possibly $t$). The Lagrangian equations (2.19) will then be obtained by substituting the resulting expressions for the $p_i$ into the second of the Hamiltonian equations. If, however, the first of the Hamiltonian equations is not thus solvable the function $S(q'', t'' \,|\, q', t')$ will not exist, and the Lagrangian function and the action principle will not exist in the usual sense. This case, the occurrence of which implies that the "velocities" $\dot{q}^i$ are not all independently specifiable, has been considered by Dirac[12] who has shown that a modified Lagrangian theory may still be constructed for it. It is of little practical importance, however, and will be ignored in this series of papers.

Much more important is the opposite case in which the momenta are not all independent, so that (2.22) cannot be solved to express the $\dot{q}^i$ in terms of the $q^i$, $p_i$ (and $t$). This case has also been considered by Dirac[12] and leads to various possibilities, some of which will be carefully studied in subsequent papers of this series. One possible consequence, for example, is that the generating function $S(q'', t'' \,|\, q', t')$, although it exists, may not define a unique trajectory [implying lack of unique solubility of (2.11)]. This would mean that many different extremal trajectories could be inserted into the right-hand side of (2.18), all leading to the same value of the action. In the present paper, however, such possibilities will be excluded.

## 3. CONSERVATION LAWS

Suppose we make a change in the representation of a physical system at any instant from a set of canonical variables $q^i(t)$, $p_i(t)$ to another set $\bar{q}^i(t)$, $\bar{p}_i(t)$. Consider

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[12] P. A. M. Dirac, Can. J. Math. **2**, 129 (1950).

the function $V$ of (1.15) which characterizes this canonical transformation. If the form of $V$, considered as a function of $q^i$, $p_i$, $\bar{q}^i$, $\bar{p}_i$, remains constant in time then, by (1.42), the generators of infinitesimal displacements in time must be equal in the two representations. That is, $\bar{H} = H$ where $H$ and $\bar{H}$ are the Hamiltonian functions for the two representations. ($H$ and $\bar{H}$ may, of course, have different functional forms.) This result also follows from the canonical invariance of Poisson brackets, equations like (2.3) being independent of the choice of representation.

If, however, the form of $V$ changes with time, so that $V$ must be regarded as having an explicit dependence on $t$, $H$ and $\bar{H}$ will no longer be equal but will be related by

$$-2(\bar{H} - H)\delta t = \bar{\delta} V. \tag{3.1}$$

If the change of representation is described by one of the generators $S_{\pm\pm}$ this equation may be replaced by

$$\bar{H} = H - \partial S_{\pm\pm}/\partial t, \tag{3.2}$$

which is a special case of the theorem at the end of Sec. 1.

It may happen that the generator is such that $\bar{H} = 0$. From the right-hand side of (3.2) we see that this will be the case if the generator satisfies a Hamilton-Jacobi equation. The new variables $\bar{q}^i$, $\bar{p}_i$ are then constant in time and, when expressed as functions of the $q^i$, $p_i$, and $t$, are known as *constants of the motion*. It is clear that the functions $S(q'', t'' \,|\, p', t')$, etc., considered in the previous section are special cases of such generators, which transform the canonical variables at an arbitrary time $t''$ back to their *constant* values at some fixed initial time $t'$.

A solution of the Hamilton-Jacobi equation gives a complete set of $2n$ independent constants of the motion. Except in very special cases, however, the Hamilton-Jacobi equation cannot be solved by finite methods, and is therefore unsuitable for the practical determination of constants of the motion. We must usually be content with a knowledge of only some of them, and for this purpose an investigation of infinitesimal changes of representation is more useful.

The change in the Hamiltonian under a canonical transformation generated by an infinitesimal $s$ is given by

$$\bar{H} = H - \partial s/\partial t, \tag{3.3}$$

which follows from (1.28) and (3.1). Now suppose that $\bar{H}$, when expressed in terms of the $\bar{q}^i$, $\bar{p}_i$, has the same functional form as does $H$ when expressed in terms of the $q^i$, $p_i$. Then, from (1.32),

$$H - (H,s) = H(\bar{q}, \bar{p}, t) = \bar{H}(\bar{q}, \bar{p}, t) = H - \partial s/\partial t,$$

or

$$\dot{s} = (s, H) + \partial s/\partial t = 0. \tag{3.4}$$

Therefore, constants of the motion may be determined by discovering those infinitesimal canonical transforma-

tions which leave the form of the Hamiltonian function invariant. A special case is provided by the Hamiltonian itself when it has no explicit dependence on the time. It then leaves itself invariant under its own infinitesimal transformations and is a constant of the motion.

Since the form of the Hamiltonian function remains invariant under an infinitesimal canonical transformation generated by a constant of the motion, the $\bar{q}^i$, $\bar{p}_i$ satisfy the same equations of motion as the $q^i$, $p_i$, and it is evident that a constant of the motion may also be regarded as the generator of an infinitesimal canonical transformation which transforms trajectories into trajectories.[13] From this point of view it is often easier to work directly from the Lagrangian than from the Hamiltonian. For example, suppose the Lagrangian function remains invariant under the transformation

$$\bar{q}^i = q^i - \delta q^i, \quad \dot{\bar{q}}^i = \dot{q}^i - \delta \dot{q}^i, \tag{3.5}$$

where the $\delta q^i$ are certain infinitesimal functions of the $q^i$ and $t$ alone. Invariance of the Lagrangian function implies invariance of the Lagrangian equations and hence also of the Hamiltonian equations, so that $\bar{q}^i$ is a trajectory if $q^i$ is. Moreover, invariances of this type are generally very easy to spot. Using the Lagrangian equations, we have

$$0 = \frac{\partial L}{\partial q^i}\delta q^i + \frac{\partial L}{\partial \dot{q}^i}\delta \dot{q}^i = \frac{d}{dt}(p_i \delta q^i), \tag{3.6}$$

so that the constant of the motion in this case is $p_i \delta q^i$. Evidently $p_i \delta q^i$ generates the transformation from the trajectory $q^i$ to the trajectory $q^i - \delta q^i$.

If the Lagrangian function has no explicit dependence on the time then the classical action must remain invariant if the whole trajectory (together with its end points) is displaced in time by a constant $\delta t$ as well as in coordinate space by the amounts $\delta q^i$ above. Using previous results, we may express this by writing

$$0 = \delta S = p''_i \delta q''^i - p'_i \delta q'^i - (H'' - H')\delta t. \tag{3.7}$$

Since $\delta t$ is arbitrary we have

$$H'' = H', \tag{3.8}$$

and

$$p''_i \delta q''^i = p'_i \delta q'^i. \tag{3.9}$$

Equations like (3.8) or (3.9) are known as *conservation laws*.

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[13] This way of looking at things enables one to use a simple argument to prove that the Poisson bracket of two constants of the motion, $F$ and $G$, is also a constant of the motion: If $F$ and $G$ are finite, render them infinitesimal through multiplication by a constant infinitesimal. Let the function $G$ generate an infinitesimal canonical transformation which transforms trajectories into trajectories. The change in $F$ under such a transformation from one trajectory to another is $\delta F = -(F,G)$. But since $F$, being a constant of the motion, is constant along both trajectories, its change $\delta F$ is also a constant; q.e.d. This result can also be obtained formally from (2.4).

## 4. QUANTUM TRANSFORMATION THEORY

Historically the quantum theory has been built up by analogy from classical dynamics. Many routes may be followed in this development, and it is somewhat a matter of taste which is chosen. In order to parallel the development of Sec. 1 as closely as possible we begin with the construction of the quantum analog of the classical Poisson bracket.

Perhaps the most elegant formal argument leading to the quantum analog is that due to Dirac[14]: Let us assume, as given, the general mathematical framework of quantum mechanics, involving linear operators, state vectors, and their adjoints, and the probability interpretation of these quantities. Real physical observables are represented in the quantum theory by Hermitian operators $F$, $G$, etc. A quantum analog for the classical Poisson bracket is expected to satisfy identities paralleling as closely as possible (1.4, 1.5, 1.6). Equation (1.4) offers no particular difficulty. However, in generalizing (1.5) we must discover a rule for defining functions of several operators, and the derivatives of such functions. Formally we may expand the classical forms of these functions in series of products of their arguments. The classical arguments can then be replaced by the corresponding quantum operators, provided we can resolve the ambiguity which arises in the ordering of these operators due to the fact that they, unlike their classical counterparts, do not necessarily commute with one another.

In this series of papers we shall have to devote considerable attention to this *ordering problem*. However, let us set it aside for the present and suppose we have the quantum analog of some simple classical observable $F$ expressed as a product of operators $F_1$, $F_2$, $\cdots$.

$$F = F_1 F_2 \cdots. \tag{4.1}$$

The differential law for this operator has the simple form

$$\delta F = [(\delta F_1)F_2 \cdots] + [F_1(\delta F_2)\cdots] + \cdots. \tag{4.2}$$

Suppose now that the variation indicated is due to an infinitesimal canonical transformation, whatever that may mean in the present context. In the quantum theory as in the classical theory we try to express this variation in the form (1.32), the only difference being that $s$ is now an infinitesimal operator. Thus

$$\delta F = -(F,s), \tag{4.3}$$

$$\delta F_i = -(F_i, s), \quad i = 1, 2 \cdots. \tag{4.4}$$

Equations (4.2, 4.3, 4.4) will be simultaneously satisfied for arbitrary $s$ if and only if the following law is satisfied:

$$(F_1 F_2, F_3) = (F_1, F_3)F_2 + F_1(F_2, F_3), \tag{4.5}$$

where $F_1$, $F_2$, $F_3$ are arbitrary operators, the order of

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[14] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, New York, 1947), third edition, §21.

the factors being now important. Equation (4.5), combined with the identity

$$(F_1,F_2) = -(F_2,F_1), \qquad (4.6)$$

implies also

$$(F_1,F_2F_3) = (F_1,F_2)F_3 + F_2(F_1,F_3). \qquad (4.7)$$

If one now considers a quantum Poisson bracket of the form $(AB,CD)$ one finds that it may be re-expressed in two different ways with the aid of (4.5) and (4.7), depending on which is used first:

$$(AB,CD) = [(A,C)D + C(A,D)]B$$
$$+ A[(B,C)D + C(B,D)] \qquad (4.8a)$$
$$= [(A,C)B + A(B,C)]D$$
$$+ C[(A,D)B + A(B,D)]. \qquad (4.8b)$$

Subtracting one form from the other, one gets

$$0 = (A,C)[B,D] - [A,C](B,D), \qquad (4.9)$$

where $[\ ]$ denotes the commutator. Equation (4.9) can hold for arbitrary operators if and only if, for any pair $A$, $B$, $(A,B)$ always stands in a constant numerical ratio to $[A,B]$. Since $[A,B]$ is anti-Hermitian if $A$ and $B$ are Hermitian, whereas $(A,B)$ must be Hermitian, the numerical constant must be imaginary. Experimental physics tells us we must set

$$(A,B) = (i\hbar)^{-1}[A,B], \qquad (4.10)$$

where $\hbar = 1.054 \times 10^{-27}$ erg sec. From (4.10) it is but a step to show that quantum Poisson brackets also satisfy the Poisson-Jacobi identity:

$$(F_1,(F_2,F_3)) + (F_2,(F_3,F_1)) + (F_3,(F_1,F_2))$$
$$= -\tfrac{1}{2}\hbar^{-2}\epsilon_{abc}(F_aF_bF_c + F_cF_bF_a$$
$$- F_aF_cF_b - F_bF_cF_a) = 0. \qquad (4.11)$$

Combining (4.3) and (4.10) we have the familiar result that an infinitesimal canonical transformation is, in the quantum theory, simply an infinitesimal unitary transformation:

$$\bar{F} = F + \delta F = F + i\hbar^{-1}[F,s] = UFU^{-1}, \qquad (4.12)$$

where

$$U = 1 - i\hbar^{-1}s, \qquad (4.13)$$

$$U^{-1} = 1 + i\hbar^{-1}s. \qquad (4.14)$$

More generally, a finite unitary transformation in the quantum theory will be expected to correspond in the classical theory to a finite canonical transformation. It should not be supposed, however, that the group of all unitary transformations in the quantum theory is isomorphic with the group of all canonical transformations in the classical theory. Such an isomorphism is prevented from existing by the ambiguity in the definition of the quantum analogs of general classical quantities,

resulting from the noncommutativity of basic operators such as $q^i$, $p_i$. In general the most that can be established is a mapping from one group into the other, which becomes one-to-one only in the classical limit $\hbar \to 0$. However, in the special cases to be considered in this series of papers, the ambiguity can be essentially removed from all physically significant quantum analogs, and a considerably stronger result can be established, namely, that there exists a *subgroup* of the full unitary group which *is* isomorphic to the group of all those canonical transformations which have any physical significance in the classical theory. This is an alternative statement of the fact that the classical theory in every case completely determines the corresponding quantum theory.

In the classical theory a canonical transformation can be regarded from two points of view, either as producing a change in the value of a physical observable $F$, as in (1.32), or as producing a change in the functional form of the observable, its value remaining fixed, as in (1.35). These alternatives have their analogs in the quantum theory. In the classical theory a change in the functional form is caused by a change of representation from one set of canonical variables to another. In the quantum theory the analogous change is in the *representative* $\langle \alpha'' | F | \alpha' \rangle$ of $F$ as the representation in terms of basic vectors $|\alpha'\rangle$ is changed. The $|\alpha'\rangle$ are orthogonal eigenvectors of a complete set of commuting Hermitian operators $\alpha_i$. If the $\alpha_i$ are subjected to a unitary transformation

$$\bar{\alpha}_i = U\alpha_i U^{-1}, \qquad (4.15)$$

the new operators $\bar{\alpha}_i$ will define an eigenbasis

$$|\bar{\alpha}'\rangle = U|\alpha'\rangle. \qquad (4.16)$$

If $U$ is given by (4.13) then the resulting change in the representative of $F$ is

$$\delta\langle \alpha'' | F | \alpha' \rangle = \langle \bar{\alpha}'' | F | \bar{\alpha}' \rangle - \langle \alpha'' | F | \alpha' \rangle$$
$$= \langle \alpha'' | (U^{-1}FU - F) | \alpha' \rangle$$
$$= -i\hbar^{-1}\langle \alpha'' | [F,s] | \alpha' \rangle$$
$$= -\langle \alpha'' | \delta F | \alpha' \rangle. \qquad (4.17)$$

It is to be noted that the eigenvalues $\bar{\alpha}'$ and $\alpha'$ are identical. Therefore here, just as in our development of the classical theory, the use of primes will have the effect of singling out particular values of the variables, independently of the representation.

The generators of finite canonical transformations in the classical theory have also their quantum analogs, *viz.*, in the "transformation functions"

$$\langle \alpha''(2) | \alpha'(1) \rangle = \langle \alpha''(1) | U^{-1} | \alpha'(1) \rangle \qquad (4.18a)$$
$$= \langle \alpha''(2) | U^{-1} | \alpha'(2) \rangle \qquad (4.18b)$$

between two sets of commuting Hermitian operators, $\alpha_i(1)$ and $\alpha_i(2)$, which are related by a finite unitary

transformation

$$\alpha_i(2) = U\alpha_i(1)U^{-1}. \tag{4.19}$$

Suppose the operators $\alpha_i(1)$ and $\alpha_i(2)$ are subjected to independent infinitesimal canonical transformations:

$$\bar{\alpha}_i(1) = \alpha_i(1) + i\hbar^{-1}[\alpha_i(1), s(1)], \tag{4.20}$$

$$\bar{\alpha}_i(2) = \alpha_i(2) + i\hbar^{-1}[\alpha_i(2), s(2)]. \tag{4.21}$$

The corresponding changes in the eigenvectors $|\alpha'(1)\rangle$, $|\alpha'(2)\rangle$ will be

$$\delta|\alpha'(1)\rangle = -i\hbar^{-1}s(1)|\alpha'(1)\rangle, \tag{4.22}$$

$$\delta|\alpha'(2)\rangle = -i\hbar^{-1}s(2)|\alpha'(2)\rangle, \tag{4.23}$$

producing a change in the transformation function of amount

$$\delta\langle\alpha''(2)|\alpha'(1)\rangle = i\hbar^{-1}\langle\alpha''(2)|[s(2)-s(1)]|\alpha'(1)\rangle. \tag{4.24}$$

Equation (4.24) is the quantum analog of the theorem at the end of Sec. 1.

In the problems usually considered (4.24) has an immediate application in the dynamical theory, just as (1.43) is applied in the classical theory to obtain the Hamilton-Jacobi equations. For the more general systems at which the present work is aimed, however, a slight modification of (4.24) will be necessary in order that the normalization of the vectors $|\alpha'(1)\rangle$ and $|\alpha'(2)\rangle$ be permitted to undergo desirable variations. We simply call attention to this fact here, postponing fuller discussion to the next section.

The question of normalization arises in the representation of an arbitrary state vector $|\psi\rangle$ as a superposition of eigenvectors $|\alpha'\rangle$, which is possible owing to the completeness condition on the operators $\alpha_i$:

$$|\psi\rangle = \int |\alpha'\rangle d\alpha' \langle\alpha'|\psi\rangle, \tag{4.25}$$

where $\int d\alpha'$ indicates an integration and/or summation over all eigenvalues $\alpha'$. The "volume element" $d\alpha'$ will generally contain a density function which serves to adjust the normalization. An explicit expression of the normalization is obtained by multiplying (4.25) on the left by $\langle\alpha''|$, which leads to

$$\langle\alpha''|\alpha'\rangle = \delta(\alpha'',\alpha'), \tag{4.26}$$

where

$$\int \delta(\alpha'',\alpha')f(\alpha')d\alpha' = f(\alpha''), \tag{4.27}$$

for arbitrary $f(\alpha')$.

## 5. QUANTUM DYNAMICS AND THE COORDINATE REPRESENTATION

Continuing the sequence of analogies to classical theory, one may base quantum dynamical theory on the

*Dynamical postulate:*

*The temporal behavior of the operators representing the observables of a physical system is determined by the unfolding-in-time of a unitary transformation.*

The infinitesimal generator of the unitary transformation $t \to t+\delta t$ will have the form $s = -H\delta t$ where $H$ is the quantum analog of the classical Hamiltonian, assuming it can be unambiguously defined. The time rate of change of any physical observable will then be given by the quantum form of (2.3).

$$\dot{F} = (i\hbar)^{-1}[F,H] + \partial F/\partial t. \tag{5.1}$$

In order to discover the appropriate quantum form for a given Hamiltonian it will be necessary to study the basic operators out of which it is constructed, in particular the operators $q^i$, $p_i$ corresponding to the classical coordinates and momenta. These operators must satisfy the commutation relations

$$[q^i, q^j] = 0, \tag{5.2}$$

$$[q^i, p_j] = i\hbar\delta_j{}^i, \tag{5.3}$$

$$[p_i, p_j] = 0, \tag{5.4}$$

corresponding to the analogous classical Poisson bracket relations. Equations (5.2) permit us to choose the $q^i$ as a set of Hermitian operators defining a complete eigenbasis. A normal notation for expressing this would be

$$q^i(t)|q'(t)\rangle = q'^i(t)|q'(t)\rangle, \tag{5.5}$$

where the dependence of the $q^i$ on the time is explicitly indicated. However, since the prime singles out a particular eigenvalue of $q^i$, independently of the time, it is more convenient to make the replacement

$$|q'(t)\rangle = |q',t\rangle, \tag{5.6}$$

and write

$$q^i|q',t\rangle = q'^i|q',t\rangle, \tag{5.7}$$

making the dependence of $q^i$ on $t$ explicit only when it is necessary to avoid confusion.

We now assume that a *natural metric* is defined in the space of the $q^i$, and choose the normalization of the $|q',t\rangle$ according to[15]

$$\langle q'',t|q',t\rangle = \delta(q'',q',t), \tag{5.8}$$

where

$$\int \delta(q'',q',t)f(q')d_tq' = f(q''), \tag{5.9}$$

for arbitrary $f(q')$, $d_tq'$ being the invariant volume element. The notation reflects the fact that the metric, and hence the normalization, may change with time. The explicit form for $d_tq'$ is

$$d_tq' = g^{\frac{1}{2}}(q',t)dq'^1 \cdots dq'^n, \tag{5.10}$$

[15] The development here follows a previous paper: B. S. DeWitt, Phys. Rev. **85**, 653 (1952).

where $g(g,t)$ is the determinant of the metric tensor. This implies

$$\delta(q'',q',t) = g^{-\frac{1}{2}}(q'',t)\delta(q''-q') \qquad (5.11a)$$

$$= g^{-\frac{1}{2}}(q',t)\delta(q''-q'), \qquad (5.11b)$$

$\delta(q''-q')$ being the ordinary $n$-dimensional delta function.

From (5.11) one may obtain the formal identities

$$(q''^i-q'^i)\delta(q'',q',t) = 0, \qquad (5.12)$$

$$\frac{\partial}{\partial q''^i}\delta(q'',q',t)$$

$$= -\frac{\partial}{\partial q'^i}\delta(q'',q',t) - \frac{1}{2}\frac{\partial}{\partial q'^i}[\ln g(q',t)]\delta(q'',q',t), \quad (5.13)$$

$$(q''^i-q'^i)\frac{\partial}{\partial q''^i}\delta(q'',q',t) = -(q''^i-q'^i)\frac{\partial}{\partial q'^i}\delta(q'',q',t)$$

$$= -\delta_j{}^i\delta(q'',q',t). \qquad (5.14)$$

From these identities it is easy to obtain the representative of the operator $p_i$ in the coordinate representation, the representative, or "matrix element," of $q^i$ being

$$\langle q'',t|q^i|q',t\rangle = q'^i\delta(q'',q',t) = q''^i\delta(q'',q',t). \quad (5.15)$$

Taking the matrix element of (5.3), we get

$$i\hbar\delta_j{}^i\delta(q'',q',t) = \int (\langle q'',t|q^i|q''',t\rangle\langle q''',t|p_j|q',t\rangle$$

$$- \langle q'',t|p_j|q''',t\rangle\langle q''',t|q^i|q',t\rangle)d_tq'''$$

$$= (q''^i-q'^i)\langle q'',t|p_j|q',t\rangle, \qquad (5.16)$$

which, in view of (5.12) and (5.14), implies

$$\langle q'',t|p_j|q',t\rangle$$

$$= -i\hbar\frac{\partial}{\partial q''^j}\delta(q'',q',t) + F_j(q'',t)\delta(q'',q',t), \quad (5.17)$$

where the $F_j(q,t)$ are certain functions of the $q^i$ and $t$. Alternative forms of (5.17) are

$$\langle q'',t|p_j|q',t\rangle$$

$$= g^{-\frac{1}{2}}(q'',t)\left[-i\hbar\frac{\partial}{\partial q''^j}+G_j(q'',t)\right]\delta(q''-q') \quad (5.18a)$$

$$= g^{-\frac{1}{2}}(q'',t)\left[i\hbar\frac{\partial}{\partial q'^j}+G_j(q',t)\right]\delta(q''-q'), \quad (5.18b)$$

where

$$G_j = F_j + \tfrac{1}{2}i\hbar\partial(\ln g)/\partial q^j. \qquad (5.19)$$

The commutation relations (5.4) will impose restrictions on the functions $F_j$. Taking the matrix element

of (5.4) and using (5.18), one gets

$$0 = \int (\langle q'',t|p_i|q''',t\rangle\langle q''',t|p_j|q',t\rangle$$

$$- \langle q'',t|p_j|q''',t\rangle\langle q''',t|p_i|q',t\rangle)d_tq'''$$

$$= g^{-\frac{1}{2}}(q',t)\left[\hbar^2\frac{\partial^2}{\partial q''^i\partial q'^j} - i\hbar G_j(q',t)\frac{\partial}{\partial q''^i} + i\hbar G_i(q'',t)\frac{\partial}{\partial q'^j}\right.$$

$$+ G_i(q'',t)G_j(q',t) - \hbar^2\frac{\partial^2}{\partial q''^j\partial q'^i} + i\hbar G_i(q',t)\frac{\partial}{\partial q''^j}$$

$$\left. - i\hbar G_j(q'',t)\frac{\partial}{\partial q'^i} - G_j(q'',t)G_i(q',t)\right]\delta(q''-q')$$

$$= -i\hbar\left[\frac{\partial}{\partial q''^i}G_j(q'',t) - \frac{\partial}{\partial q''^j}G_i(q'',t)\right]\delta(q'',q',t)$$

$$= -i\hbar\left[\frac{\partial}{\partial q''^i}F_j(q'',t) - \frac{\partial}{\partial q''^j}F_i(q'',t)\right]\delta(q'',q',t) \qquad (5.20)$$

which implies[16]

$$F_i = \partial F/\partial q^i \qquad (5.21)$$

for some function $F$ of the $q^i$ and $t$.

A final restriction on $F$ is imposed by the Hermitian condition on the $p_i$. We must have

$$\langle q'',t|p_i|q',t\rangle^* = \langle q',t|p_i|q'',t\rangle. \qquad (5.22)$$

Insertion of (5.17) into (5.22) and use of the identity (5.13) yields the condition

$$F^\dagger = F + \tfrac{1}{2}i\hbar \ln g, \qquad (5.23)$$

which implies that $F$ has the form

$$F = -\Phi - \tfrac{1}{4}i\hbar \ln g, \qquad (5.24)$$

where $\Phi$ is some real function of the $q^i$ and $t$. The dependence of the representative of $p_i$ on $\Phi$ may be removed by performing the unitary phase transformation

$$\bar{p}_i = e^{-(i/\hbar)\Phi}p_i e^{(i/\hbar)\Phi} = p_i + \partial\Phi/\partial q^i, \qquad (5.25)$$

or alternatively by redefining the basis vectors according to

$$\overline{|q',t\rangle} = e^{(i/\hbar)\Phi}|q',t\rangle. \qquad (5.26)$$

The transformation (5.26) simply changes the phase of the eigenvector $|q',t\rangle$ by the amount $\hbar^{-1}\Phi(q',t)$. Since this phase was arbitrary to begin with, we may assume that the adjustment (5.26) has already been made and write the representative of $p_i$ in the standard form

$$\langle q'',t|p_i|q',t\rangle$$

$$= -i\hbar\left\{\frac{\partial}{\partial q''^i} + \frac{1}{4}\left[\frac{\partial}{\partial q''^i}\ln g(q'',t)\right]\right\}\delta(q'',q',t). \quad (5.27)$$

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[16] There is no difficulty in defining the derivative of an operator function of commuting variables.

A more conventional representation of the $q^i$, $p_i$ is in terms of differential operators acting on the representative, or "wave function"

$$\psi(q',t) = \langle q',t | \psi \rangle \qquad (5.28)$$

of an arbitrary state $|\psi\rangle$. The differential form $F_{q'}(t')$ of an operator $F$ is defined by

$$F_{q'}(t')\psi(q',t') = \langle q',t' | F(t') | \psi \rangle, \qquad (5.29)$$

and in particular,

$$q^i{}_{q'} = q'^i, \qquad (5.30)$$

$$p_{iq'} = -i\hbar [\partial/\partial q'^i + \tfrac{1}{4}(\ln g')_{,i}]. \qquad (5.31)$$

Here we use the abbreviations

$$f' \equiv f(q',t'), \qquad (5.32)$$

$$f_{,i} \equiv \partial f/\partial q^i, \qquad (5.33)$$

$$f'_{,i} \equiv \partial f(q',t')/\partial q'^i, \qquad (5.34)$$

where $f$ is an arbitrary function of the $q^i$ and $t$. The prime is henceforth understood as occurring on the $q^i$ and $t$ together unless otherwise indicated. Repeated differentiation is denoted by additional indexes after the comma.

The assumption that coordinate space possesses a natural metric means that special importance is attached to point transformations in this space. We proceed to examine these transformations. Here we run into a slight notational problem. In the classical theory a point transformation is a canonical transformation, (1.25). In the quantum theory we may expect it to be describable as a unitary transformation:

$$\bar{q}^i = \bar{q}^i(q,t) = U q^i U^{-1}. \qquad (5.35)$$

If we now follow our usual convention, according to which a prime singles out a particular eigenvalue independently of the representation, we shall have $\bar{q}'^i = q'^i$ and $|\bar{q}',t'\rangle = U|q',t'\rangle$. But if we do this, a given eigenvalue will refer to different points of coordinate space, depending on the representation; $\bar{q}'$ will refer to that point whose coordinate values in the new representation are identical with the coordinate values of the original point in the original coordinate system. This raises difficulties in eigenvector normalization, since the normalization condition (5.8) and (5.9), depending on the invariant volume element, is designed to be independent of the coordinate system chosen. Therefore, it is more convenient to regard the prime as singling out a particular *point* of coordinate space[17] and write

$$\bar{q}'^i = \bar{q}^i(q',t'), \qquad (5.36)$$

$$|\bar{q}',t'\rangle = |q',t'\rangle, \qquad (5.37)$$

$$\bar{q}^i | q',t' \rangle = \bar{q}'^i | q',t' \rangle. \qquad (5.38)$$

Under a point transformation the determinant of the metric tensor transforms according to

$$\bar{g} = |\partial q/\partial\bar{q}|^2 g, \qquad (5.39)$$

where $|\partial q/\partial\bar{q}|$ denotes the coordinate Jacobian. Therefore

$$\ln\bar{g} = \ln g + 2\ln|\partial q/\partial\bar{q}|, \qquad (5.40)$$

and

$$\overline{(\ln g)}_{,i} = \partial(\ln g)/\partial\bar{q}^i + 2|\partial\bar{q}/\partial q|\,\partial|\partial q/\partial\bar{q}|/\partial\bar{q}^i$$

$$= (\partial q^j/\partial\bar{q}^i)(\ln g)_{,j} + 2(\partial q^j/\partial\bar{q}^i)_{,j}. \qquad (5.41)$$

Equation (5.41) may be used with (5.31) to obtain the point transformation law for the momenta:

$$\bar{p}_{iq'} = -i\hbar[\partial/\partial\bar{q}'^i + \tfrac{1}{4}\overline{(\ln g')}_{,i}]$$

$$= -i\hbar(\partial q'^j/\partial\bar{q}'^i)[\partial/\partial q'^j + \tfrac{1}{4}(\ln g')_{,j}]$$

$$\qquad -\tfrac{1}{2}i\hbar(\partial q'^j/\partial\bar{q}'^i)_{,j}$$

$$= \tfrac{1}{2}\{p_{jq'}, \partial q'^j/\partial\bar{q}'^i\}, \qquad (5.42)$$

or

$$\bar{p}_i = \tfrac{1}{2}\{p_j, \partial q^j/\partial\bar{q}^i\}, \qquad (5.43)$$

where $\{\ \}$ denotes the anticommutator. Equation (5.43) is the quantum generalization of the last of (1.25). The symmetrization effected by the anticommutator insures that the transformation leaves the Hermitian character of the $p_i$ unchanged.[18]

An infinitesimal point transformation is given by

$$U = 1 - \tfrac{1}{2}i\hbar^{-1}\{p_i, \delta q^i\}, \qquad (5.44)$$

$$\bar{q}^i = U q^i U^{-1} = q^i - \delta q^i, \qquad (5.45)$$

$$\bar{p}_i = U p_i U^{-1} = p_i + \tfrac{1}{2}\{p_j, \delta q^j{}_{,i}\}, \qquad (5.46)$$

where the $\delta q^i$ are arbitrary infinitesimal functions of the $q$'s and $t$ [see (1.31), (4.13)].[19] The vector $U(t')|q',t'\rangle$ is an eigenvector of $\bar{q}^i(t')$ corresponding to the eigenvalue $q'^i$. This eigenvalue refers, in the coordinate system $\bar{q}$, to a point which in the coordinate system $q$ has the coordinate values $q'^i + \delta q'^i$. Therefore $U(t')|q',t'\rangle$ must be proportional to the eigenvector $|q'+\delta q',t'\rangle$:

$$U(t')|q',t'\rangle = A'^{\frac{1}{2}}|q'+\delta q',t'\rangle. \qquad (5.47)$$

The proportionality constant $A'^{\frac{1}{2}}$ is not necessarily equal to unity since the operator $U$ refers the normalization back to that obtaining at the point $q'$, whereas the normalization required at the point $q'+\delta q'$ will generally be different. $A'$ is readily evaluated by considering the

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[17] This also avoids difficulties arising from coordinate transformations for which the spectra of $q^i$ and $\bar{q}^i$ are not identical.

[18] Any other method of symmetrization would lead to the same result. For example, one might expand $\partial q^j/\partial\bar{q}^i$ in a power series in the $q$'s. The operator $p_j$ could then be inserted between the $q$'s in any symmetrical fashion in each term of the series. The result of commuting $p_j$ symmetrically to the left and to the right through the $q$'s would be to produce two terms proportional to $\hbar$ which cancel each other, leaving (5.43).

[19] The unitary operator describing a finite point transformation has the general form $U = \exp[-\tfrac{1}{2}i\hbar^{-1}\{p_i, \Lambda^i\}]$ where the $\Lambda^i$ are finite functions of the $q$'s and $t$.

representative of an arbitrary state vector $|\psi\rangle$. We may write

$$A'^{\frac{1}{2}*}(\langle q',t'|\psi\rangle+\delta q'^i\partial\langle q',t'|\psi\rangle/\partial q'^i)$$
$$=A'^{\frac{1}{2}*}\langle q'+\delta q',t'|\psi\rangle=\langle q',t'|U^{-1}(t')|\psi\rangle$$
$$=\langle q',t'|\psi\rangle+\tfrac{1}{2}i\hbar^{-1}\langle q',t'|\{p_i,\delta q^i\}|\psi\rangle$$
$$=\langle q',t'|\psi\rangle+\delta q'^i\partial\langle q',t'|\psi\rangle/\partial q'^i$$
$$+\tfrac{1}{2}[\delta q'^i{}_{,i}+\tfrac{1}{2}(\ln g')_{,i}\delta q'^i]\langle q',t'|\psi\rangle. \quad (5.48)$$

Comparison of the first and last lines shows that

$$A=1+\delta q^i{}_{.i}, \quad (5.49)$$

where the dot followed by an index denotes the covariant derivative. The physical meaning of (5.49) is quite clear. If the points of any small region of coordinate space are subjected to displacements $\delta q^i$, the volume of the shifted region is increased by the factor $A$. Volume is conserved only if the displacements are divergenceless. This applies specifically to the displacement of the invariant volume element, which is effected by the operator $U$.

A similar situation exists in regard to displacements in time. The appropriate unitary operator in this case is

$$V=1+i\hbar^{-1}H\delta t, \quad (5.50)$$

where $\delta t$ is an arbitrary infinitesimal function of the time. The vector $V(t')|q',t'\rangle$ is an eigenvector of the operators $V(t')q^i(t')V^{-1}(t')=q^i(t'+\delta t')$ corresponding to the eigenvalues $q'^i$.[20] Therefore

$$V(t')|q',t'\rangle=B'^{\frac{1}{2}}|q',t'+\delta t'\rangle. \quad (5.51)$$

The normalization constant is determined in this case by the representatives (5.15) and (5.27) of the $q^i$ and $p_i$, respectively, and by the relation

$$\delta(q'',q',t+\delta t)=\delta(q'',q',t)+\delta t\partial\delta(q'',q',t)/\partial t$$
$$=[1-\tfrac{1}{2}\delta t\partial\ln g(q'',t)/\partial t]\delta(q'',q',t) \quad (5.52)$$

which follows from (5.11). We have first of all

$$\langle q'',t|q^i(t)|q',t\rangle$$
$$=\langle q'',t|V^{-1}(t)V(t)q^i(t)V^{-i}(t)V(t)|q',t\rangle$$
$$=B^{\frac{1}{2}*}(q'',t)B^{\frac{1}{2}}(q',t)\langle q'',t+\delta t|q^i(t+\delta t)|q',t+\delta t\rangle$$
$$=B^{\frac{1}{2}*}(q'',t)B^{\frac{1}{2}}(q',t)q''^i\delta(q'',q',t+\delta t)$$
$$=|B(q'',t)|[1-\tfrac{1}{2}\delta t\partial\ln g(q'',t)/\partial t]$$
$$\times\langle q'',t|q^i(t)|q',t\rangle, \quad (5.53)$$

which implies

$$B=1+[\tfrac{1}{2}\partial(\ln g)/\partial t+2i\omega]\delta t, \quad (5.54)$$

[20] These eigenvalues are the coordinate values of a point at the time $t'+\delta t'$. A point at the original time $t'$ having the same coordinate values ought not, strictly speaking, to be called the *same* point, because (a) we have permitted the use of "moving" coordinate systems by allowing our point transformations to be time dependent, and (b) we have admitted the possibility that the metric structure of the coordinate space may vary with time. Under such circumstances it becomes somewhat meaningless to compare two points at different times.

where $\omega$ is some real function of the $q$'s and $t$. Secondly,

$$\langle q'',t|p_i(t)|q',t\rangle$$
$$=-i\hbar B^{\frac{1}{2}*}(q'',t)B^{\frac{1}{2}}(q',t)$$
$$\times\left\{\frac{\partial}{\partial q''^i}+\frac{1}{4}\left[\frac{\partial}{\partial q''^i}\ln g(q'',t+\delta t)\right]\right\}\delta(q'',q',t+\delta t)$$
$$=-i\hbar\left\{\frac{\partial}{\partial q''^i}+\frac{1}{4}\left[\frac{\partial}{\partial q''^i}\ln g(q'',t)\right]\right\}$$
$$\times|B(q',t)|\delta(q'',q',t+\delta t)$$
$$+i\hbar\left[\frac{\partial}{\partial q''^i}B^{\frac{1}{2}*}(q'',t)-\tfrac{1}{4}\delta t\frac{\partial^2\ln g(q'',t)}{\partial t\partial q''^i}\right]\delta(q'',q',t)$$
$$=\langle q'',t|p_i(t)|q',t\rangle$$
$$+\hbar\delta t[\partial\omega(q'',t)/\partial q''^i]\delta(q'',q',t), \quad (5.55)$$

which implies

$$\omega_{,i}=0. \quad (5.56)$$

We may set $\omega=0$ by introducing a new representation

$$\overline{|q',t'\rangle}=\exp\left(i\int^{t'}\omega dt\right)|q',t'\rangle. \quad (5.57)$$

Since $\omega$ is simply a numerical function of the time, this transformation leaves the representatives of the $q^i$, $p_i$ unchanged, and we assume it already to have been carried out.

The change in the representative of an arbitrary state vector $|\psi\rangle$ under a displacement in time may then be expressed in the form

$$\langle q',t'+\delta t'|\psi\rangle=B'^{-\frac{1}{2}}\langle q',t'|V^{-1}(t')|\psi\rangle$$
$$=[1-\tfrac{1}{4}(\partial\ln g'/\partial t')\delta t']\langle q',t'|\psi\rangle$$
$$+(i\hbar)^{-1}\langle q',t'|H(t')|\psi\rangle\delta t', \quad (5.58)$$

which leads to the Schrödinger equation for the wave function,

$$i\hbar\psi_{.t'}(q',t')=H_{q'}(t')\psi(q',t'), \quad (5.59)$$

the dot followed by a $t$ denoting *conservative* differentiation with respect to the time:

$$\psi_{.t}\equiv\partial\psi/\partial t+\tfrac{1}{4}(\partial\ln g/\partial t)\psi. \quad (5.60)$$

When the metric is allowed to vary with time such a modified derivative is required in order to insure conservation of probability, as expressed by the time invariance of the integral

$$\int|\psi(q',t')|^2d_{t'}q'=\langle\psi|\psi\rangle. \quad (5.61)$$

We may finally write down the appropriate generalization of (4.24) for the case of the dynamical transformation function $\langle q'',t''|q',t'\rangle$. Using the symbol $\delta$ now

to denote the operation

$$\delta\psi \equiv \psi_{,i}\delta q^i + \tfrac{1}{2}\psi \delta q^i_{,i} + \psi_{,t}\delta t, \qquad (5.62)$$

we have

$$\delta\langle q'',t''|q',t'\rangle = i\hbar^{-1}\langle q'',t''|[\tfrac{1}{2}\{p_i(t''),\delta q^i(t'')\}$$

$$-H(t'')\delta t'' - \tfrac{1}{2}\{p_i(t'),\delta q^i(t')\} + H(t')\delta t']|q',t'\rangle, \quad (5.63)$$

which has an obvious analogy with (2.8b).

It is possible to push the analogy even further by introducing a quantum analog for the classical action function. This is done with the aid of the concept of *well-ordered* operator functions.[21] Let $f(q'',t''|q',t')$ be an arbitrary function of the $q''$, $t''$, $q'$, $t'$. The operator

$$f(q(t''),t''|q(t'),t')$$

$$\equiv \int d_{t''}q'' \int d_{t'}q'|q'',t''\rangle f(q'',t''|q',t')\langle q',t'|, \quad (5.64)$$

is said to be the well-ordered operator form of $f(q'',t''|q',t')$. If $f(q'',t''|q',t')$ can be expanded as a power series in the $q''^i$, $q'^i$, its well-ordered operator form is obtained simply by replacing the $q''^i$, $q'^i$, respectively, by $q^i(t'')$, $q^i(t')$ in a *time-ordered* fashion. Any operator $F$ may be expressed as a well-ordered operator $F(q(t''),t''|q(t'),t')$, the associated function being simply its matrix element:

$$F(q'',t''|q',t') = \langle q'',t''|F|q',t'\rangle. \qquad (5.65)$$

In practice a given operator is generally expressed in a form which is not time ordered to begin with. To obtain it in its well-ordered form it is necessary to take into account the commutation effects of permuting its various components.

The quantum analog of the classical action is the well-ordered operator form of a function $\mathcal{S}(q'',t''|q',t')$ defined by

$$\langle q'',t''|q',t'\rangle = (g''g')^{-\frac{1}{4}}\exp[i\hbar^{-1}\mathcal{S}(q'',t''|q',t')]. \quad (5.66)$$

Using (5.62) one has

$$\delta\langle q'',t''|q',t'\rangle$$

$$= i\hbar^{-1}[(\partial\mathcal{S}/\partial q''^i)\delta q''^i - \tfrac{1}{2}i\hbar\delta q''^i_{,i} + (\partial\mathcal{S}/\partial t'')\delta t''$$

$$+ (\partial\mathcal{S}/\partial q'^i)\delta q'^i - \tfrac{1}{2}i\hbar\delta q'^i_{,i} + (\partial\mathcal{S}/\partial t')\delta t']\langle q'',t''|q',t'\rangle$$

$$= i\partial^{-1}\langle q'',t''|[\delta\mathcal{S}(q(t''),t''|q(t'),t')$$

$$- \tfrac{1}{2}i\hbar\delta q^i_{,i}(t'') - \tfrac{1}{2}i\hbar\delta q^i_{,i}(t')]|q',t'\rangle. \quad (5.67)$$

Comparison with (5.63) yields

$$\left.\begin{array}{l} p_i(t'') = \partial\mathcal{S}(q(t''),t''|q(t'),t')/\partial q^i(t''), \\ p_i(t') = -\partial\mathcal{S}(q(t''),t''|q(t'),t')/\partial q^i(t'), \end{array}\right\} \quad (5.68)$$

$$\left.\begin{array}{l} H(t'') = -\partial\mathcal{S}(q(t''),t''|q(t'),t')/\partial t'', \\ H(t') = \partial\mathcal{S}(q(t''),t''|q(t'),t')/\partial t', \end{array}\right\} \quad (5.69)$$

which are the analogs of the classical Hamilton-Jacobi

[21] P. A. M. Dirac, reference 14, §32. This famous section of Dirac's book has been phenomenally fruitful in its stimulation of the modern developments of the action principle.

equations. The derivatives on the right-hand sides must, be taken with $\mathcal{S}$ in its well-ordered form.

The operator $\mathcal{S}$ is generally non-Hermitian, in spite of the fact that its variation $\delta\mathcal{S}$ *is* Hermitian when the displacements $\delta q^i$ are chosen independent of the $q$'s so as to commute with everything. In his development of the theory of quantized fields from a single dynamical principle Schwinger[4] assumes the existence of an Hermitian operator $S$ which, when its components are ordered in some prescribed manner, possesses the same variation as $\mathcal{S}$ with $q$-independent $\delta q^i$. From the composition law

$$\delta\langle q'',t''|q',t'\rangle = \int d_{t'''}q'''(\delta\langle q'',t''|q''',t'''\rangle\langle q''',t'''|q',t'\rangle$$

$$+ \langle q'',t''|q''',t'''\rangle\delta\langle q''',t'''|q',t'\rangle)$$

$$= i\hbar^{-1}\langle q'',t''|[\delta\mathcal{S}(q(t''),t''|q(t'''),t''')$$

$$+ \delta\mathcal{S}(q(t'''),t'''|q(t'),t')]|q',t'\rangle. \quad (5.70)$$

Schwinger infers that $S$ may be chosen so as to satisfy[22]

$$S(t''|t') = S(t''|t''') + S(t'''|t'), \qquad (5.71)$$

and hence may be expressed in the form

$$S(t''|t') = \int_{t'}^{t''} L\,dt, \qquad (5.72)$$

where $L$ is a quantum analog of the classical Lagrangian function. While such an operator certainly exists in the cases Schwinger considers, namely, interacting fields possessing a Lagrangian which never involves any one field more than quadratically, it is questionable, because of operator ordering complications, whether the same is true for the nonlinear systems of primary interest in the present investigation. The difficulties will be apparent after we have constructed the explicit Hamiltonian operator for a special case.

## 6. SPECIAL SYSTEM

As stated in the introduction, the prototype for the systems to be covered by the present analysis is the system consisting of a nonrelativistic particle moving in a curved space of $n$ dimensions. The Lagrangian for this system has the general form

$$L \equiv \tfrac{1}{2}g_{ij}\dot{q}^i\dot{q}^j + a_i\dot{q}^i - v, \qquad (6.1)$$

where the $g_{ij}(=g_{ji})$, $a_i$, $v$ are functions of the $q$'s and possibly also of the time $t$. In the case of an actual particle moving in three dimensions $a_i$ and $v$ may be the vector and scalar potentials, respectively, describing the effect of an impressed electromagnetic field. In general, however, $a_i$ and $v$ will not have such a specialized significance.

[22] The operator $S$ does *not* satisfy a relation of this type, although its variation does.

The form (6.1) embraces (at least approximately) all known physical systems which satisfy Bose statistics and possess a classical analog. It may be regarded as an invariant under point transformations,[23]

$$q^i = q^i(\bar{q},t),\tag{6.2}$$

provided one imposes the transformation laws

$$\bar{g}_{ij} = \frac{\partial q^k}{\partial \bar{q}^i}\frac{\partial q^l}{\partial \bar{q}^j}g_{kl},\tag{6.3}$$

$$\bar{a}_i = \frac{\partial q^j}{\partial \bar{q}^i}\left(a_j + g_{jk}\frac{\partial q^k}{\partial t}\right),\tag{6.4}$$

$$\bar{v} = v - a_i\frac{\partial q^i}{\partial t} - \tfrac{1}{2}g_{ij}\frac{\partial q^i}{\partial t}\frac{\partial q^j}{\partial t}.\tag{6.5}$$

The form is also invariant under phase transformations

$$\bar{L} = L + d\Phi/dt,\tag{6.6}$$

provided $a_i$ and $v$ are made to transform according to

$$\bar{a}_i = a_i + \Phi_{,i},\tag{6.7}$$

$$\bar{v} = v - \partial\Phi/\partial t.\tag{6.8}$$

The equations of motion which follow from the Lagrangian function (6.1) are

$$q_{ij}\ddot{q}^j + [jk,i]\dot{q}^j\dot{q}^k + (\partial g_{ij}/\partial t - f_{ij})\dot{q}^j$$
$$+ \partial a_i/\partial t + v_{,i} = 0,\tag{6.9}$$

where

$$[jk,i] \equiv \tfrac{1}{2}(g_{ij,k} + g_{ik,j} - g_{jk,i}),\tag{6.10}$$

$$f_{ij} \equiv a_{j,i} - a_{i,j}.\tag{6.11}$$

These equations are evidently invariant in form under point and phase transformations. In the cases of greatest interest, which will eventually be studied in this series, there exist also other groups of transformations under which these equations remain invariant. When such other transformation groups exist the matrix $(g_{ij})$ is generally singular. We do not consider these cases in the present paper, but assume that $(g_{ij})$ is nonsingular and possesses an inverse $(g^{ij})$ satisfying

$$g^{ik}g_{kj} = \delta_j{}^i.\tag{6.12}$$

For a particle moving in a curved space, $g_{ij}$ is the metric of the space (up to an arbitrary constant factor). We extend this interpretation and assume quite generally that $g_{ij}$ is the natural metric for the space of the $q^i$, even when the $q^i$ are field amplitudes, nondenumerably infinite in number. Thus we may therefore eventually be dealing with the Riemannian geometry of a space having a nondenumerable infinity of dimensions.

The momenta of the canonical formalism are given in the present case by

$$p_i = \partial L/\partial \dot{q}^i = g_{ij}\dot{q}^j + a_i.\tag{6.13}$$

Since $(g_{ij})$ is nonsingular these equations may be solved to express the "velocities" in terms of the momenta:

$$\dot{q}^i = g^{ij}(p_j - a_j).\tag{6.14}$$

The Hamiltonian then becomes

$$H = p_i\dot{q}^i - L = \tfrac{1}{2}g^{ij}(p_i - a_i)(p_j - a_j) + v.\tag{6.15}$$

The action function $S(q'',t''|q',t')$ may be obtained either by solving the equations of motion (6.9) and substituting into the integral $\int L dt$, or by solving the Hamilton-Jacobi equations

$$\frac{\partial S}{\partial t''} + \tfrac{1}{2}g''^{ij}\left(\frac{\partial S}{\partial q''^i} - a''_i\right)\left(\frac{\partial S}{\partial q''^j} - a''_j\right) + v'' = 0,\tag{6.16}$$

$$-\frac{\partial S}{\partial t'} + \tfrac{1}{2}g'^{ij}\left(-\frac{\partial S}{\partial q'^i} - a'_i\right)\left(-\frac{\partial S}{\partial q'^j} - a'_j\right) + v' = 0.\tag{6.17}$$

We assume that the $g_{ij}$, $a_i$, $v$ together with their first and second derivatives are continuous functions of the $q^i$ and $t$. The quantities appearing in (6.16) may be expanded about the point $q',t'$, giving
$S(q'',t''|q',t')$

$$\begin{aligned}
= (t''-t')^{-1}\{&\tfrac{1}{2}g'_{ij}(q''^i-q'^i)(q''^j-q'^j)\\
&+ \tfrac{1}{12}(g'_{ij,k} + g'_{jk,i} + g'_{ki,j})(q''^i-q'^i)(q''^j-q'^j)\\
&\times (q''^k-q'^k) + (1/72)[g'_{ij,kl} + g'_{ik,lj} + g'_{il,jk}\\
&+ g'_{kl,ij} + g'_{lj,ik} + g'_{jk,il} - g'^{mn}([ij,m]'[kl,n]'\\
&+ [ik,m]'[lj,n]' + [il,m]'[jk,n]')]\\
&\times (q''^i-q'^i)(q''^j-q'^j)(q''^k-q'^k)(q''^l-q'^l)\\
&+ o(q''-q')^5\} + a'_i(q''^i-q'^i)\\
&+ \tfrac{1}{4}(a'_{i,j} + a'_{j,i} + \partial g'_{ij}/\partial t')(q''^i-q'^i)(q''^j-q'^j)\\
&- (a'^ia'_i + v')(t''-t') + o(q''-q')^3\\
&+ o[(t''-t')(q''-q')] + o(t''-t')^2,\end{aligned}\tag{6.18}$$

where $a^i = g^{ij}a_j$.

As a preliminary to the quantum-mechanical developments of the next section it is useful to examine the present system from a statistical viewpoint. Suppose we have an ensemble of a large number $N$ of such systems, all identical, described by a distribution function $f(q,p,t)$ such that $Nf(q,p,t)dq^1\cdots dq^n dp_1\cdots dp_n$ represents the number of systems having coordinates in the range $dq^1\cdots dq^n$ at $q$ and momenta in the range $dp_1\cdots dp_n$ at $p$, at the time $t$. Since $dq^1\cdots dq^n dp_1\cdots dp_n$ is a canonical invariant[9] and since the number of systems remains constant, $f(q,p,t)$ must have vanishing total time derivative. Written in the form

$$(f,H) + \partial f/\partial t = 0,\tag{6.19}$$

this statement becomes Liouville's conservation

[23] If the point transformation is expressed in the form $\bar{q}^i = \bar{q}^i(q,t)$ then the derivatives $\partial q^i/\partial t$ may be replaced by $-(\partial q^i/\partial \bar{q}^j)\partial \bar{q}^j/\partial t$.

theorem.[24] It may also be written in the integral form

$$\int f(q,p,t)dq^1\cdots dq^n dp_1\cdots dp_n=1. \qquad (6.20)$$

Instead of asking for the number of systems in the range $dq^1\cdots dq^n dp_1\cdots dp_n$, and thereby specifying the trajectories of these systems by means of initial conditions $q^i$, $p_i$, one may also ask for the number of systems having trajectories specified by means of certain end-point conditions. Thus, one may work with a function $F(q'',t''|q',t')$ such that $NF(q'',t''|q',t')d_{t''}q''d_{t'}q'$ represents the number of systems having coordinates in the volume element $d_{t'}q'$ at $q'$, $t'$ and in the volume element $d_{t''}q''$ at $q''$, $t''$. From (2.8b) and (5.10),

$$F(q'',t''|q',t')$$
$$=g''^{-\frac12}D(q'',t''|q',t')g'^{-\frac12}f(q',p'(q'',t''|q',t'),t'), \quad (6.21)$$

where

$$p'_i(q'',t''|q',t')=-\partial S(q'',t''|q',t')/\partial q'^i, \quad (6.22)$$

$$D=|D_{ji}|, \qquad (6.23)$$

$$D_{ji}=\frac{\partial p'_i}{\partial q''^j}=-\frac{\partial^2 S}{\partial q''^j\partial q'^i}. \qquad (6.24)$$

The determinant $D$, which is simply the Jacobian involved in changing the specification of the trajectory from the variables $q'$, $p'$ to the variables $q'$, $q''$, was first introduced by Van Vleck.[25] It satisfies an important conservation law, namely,

$$\partial D/\partial t''+\partial(\dot q''^i D)/\partial q''^i=0, \qquad (6.25)$$

$$\dot q''^i\equiv g''^{ij}(p''_j-a''_j)=g''^{ij}[(\partial S/\partial q''^j)-a''_j], \quad (6.26)$$

which follows from the insertion of (6.21) into the necessary conservation law

$$g''^{-\frac12}\partial(g''^{\frac12}F)/\partial t''+g''^{-\frac12}\partial(g''^{\frac12}\dot q''^i F)/\partial q''^i=0, \quad (6.27)$$

together with use of the identity

$$\partial p'_j/\partial t''+\dot q''^i\partial p'_j/\partial q''^i=0, \qquad (6.28)$$

which can be obtained either by differentiating (6.16)

[24] Liouville, J. math. 3, 349 (1838). Any distribution function may evidently be used to generate an infinitesimal canonical transformation which changes trajectories into trajectories. The resulting change may be described as a "rotational" displacement of the phase-space trajectories in the regions where the distribution function is nonvanishing. Since an actual distribution function is never negative the "rotation" is always in the same sense.

[25] J. H. Van Vleck, Proc. Natl. Acad. Sci. 14, 178 (1928). This delightful paper extends the central idea of the WKB method and shows explicitly how quantum mechanics with its statistical interpretation passes asymptotically to the classical theory in the Correspondence Principle limit $\hbar\to 0$. Van Vleck considers the general case in which the variables $q''^i$, $p''_i$ are referred back to an arbitrary canonical set $\alpha'$, $\beta'$ and not merely to the $q'^i$, $p'_i$. If the $\alpha'$ are chosen as the action variables for a multiply-periodic conservative system, the asymptotic equivalence of the stationary state matrix elements of an arbitrary operator to the Fourier amplitudes of the corresponding classical quantity then follows immediately from his work.

with respect to $q'^i$ or by observing that the $p'_i$ may be regarded as constants of the motion, i.e., the *fixed* values of the momenta at an initial time $t'$. Equation (6.25) may also be derived directly, without appeal to the conservation law (6.27), by differentiating (6.28) with respect to $q''^i$, multiplying by $D^{-1ji}$ where

$$D^{-1ik}D_{kj}=\delta_j{}^i, \qquad (6.29)$$

and using the theorem

$$|A|^{-1}\delta|A|=\mathrm{tr}(A^{-1}\delta A), \qquad (6.30)$$

which holds for an arbitrary nonsingular matrix $A$. In this way one may derive (6.27) instead of using it as a starting point.

If the Lagrangian (6.1) is regarded literally as describing a particle subject to forces derived from vector and scalar potentials in a curved $n$-dimensional space, then the distribution function $F(q'',t''|q',t')$ describes the motion of an ensemble of such particles. If $F(q'',t''|q',t')$ is nonvanishing only over a small range of the variables $q'^i$ and $q''^i$, then the ensemble has the form of a cluster or "packet," the motion of which approximates that of a single particle. The density of particles in the packet is $N\rho''$ where

$$\rho''=\rho(q'',t'')=\int F(q'',t''|q',t')d_{t'}q', \qquad (6.31)$$

satisfying the conservation laws

$$\int \rho''d_{t''}q''=1, \qquad (6.32)$$

$$g''^{-\frac12}\partial(g''^{\frac12}\rho'')/\partial t''+(\rho''\langle\dot q''^i\rangle_{Av})_{.i}=0, \qquad (6.33)$$

where the dot denotes covariant differentiation with respect to the $q''^i$, and where

$$\rho''\langle\dot q''^i\rangle_{Av}=\int \dot q''^i F d_{t'}q'. \qquad (6.34)$$

In the next section we shall need the first few terms in the explicit expansion of the Van Vleck determinant. Using the expansion (6.18) one finds

$$D_{ji}=(t''-t')^{-1}\{g'_{ji}+[jk,i]'(q''^k-q'^k)$$
$$+\tfrac16[[kl,i]'_{,j}+[lj,i]'_{,k}+[kj,i]'_{,l}$$
$$-g'^{mn}([ij,m]'[kl,n]'+[ik,m]'[lj,n]'$$
$$+[il,m]'[jk,n]')]$$
$$\times(q''^k-q'^k)(q''^l-q'^l)+o(q''-q')^3\}$$
$$+\tfrac12(\partial g'_{ji}/\partial t'+f'_{ji})+o(q''-q')+o(t''-t'). \quad (6.35)$$

Then, using the matrix theorem

$$|A+B|=|A||1+A^{-1}B|$$
$$=|A|\{1+\mathrm{tr}(A^{-1}B)+\tfrac12[\mathrm{tr}(A^{-1}B)]^2$$
$$-\tfrac12\mathrm{tr}(A^{-1}B)^2+\cdots\}, \qquad (6.36)$$

which may be obtained by replacing $A$ by $1+A^{-1}B$ in the integrated form of (6.30),

$$|A| = e^{\mathrm{tr}\ln A}, \tag{6.37}$$

and expanding both the logarithm and exponential, one finds

$$
\begin{aligned}
D(q'',&t''|q',t') \\
&= (t''-t')^{-n}g''^{\frac{1}{2}}g'^{\frac{1}{2}}\{1+\tfrac{1}{6}R'_{ij}(q''^{i}-q'^{i})(q''^{j}-q'^{j}) \\
&\quad + o(q''-q')^3 + o[(t''-t')(q''-q')] \\
&\hspace{4cm} + o(t''-t')^2\}, \quad (6.38)
\end{aligned}
$$

where

$$R_{ij} = -g^{kl}R_{ikjl}$$

$$
\begin{aligned}
R_{ikjl} = \tfrac{1}{2}(g_{ij,kl} - g_{il,kj} - g_{kj,il} + g_{kl,ij}) \\
+ g^{mn}([ij,m][kl,n] - [kj,m][il,n]). \quad (6.39)
\end{aligned}
$$

The $R_{ikjl}$ are the components of the *Riemann tensor*. We have defined $R_{ij}$ in such a way that the scalar

$$R = g^{ij}R_{ij} \tag{6.40}$$

is positive for a space of positive curvature.[26]

In (6.38) terms linear in $(q''^{i}-q'^{i})$ and $(t''-t')$ inside the curly brackets have been removed by replacing the factor $g'$, which would normally appear in front as a result of a straightforward application of (6.36) to (6.35), by the factor

$$
\begin{aligned}
g''^{\frac{1}{2}}g'^{\frac{1}{2}} = g'[1 &+ g'^{-\frac{1}{2}}(g'^{\frac{1}{2}})_{,i}(q''^{i}-q'^{i}) \\
&+ g'^{-\frac{1}{2}}(\partial g'^{\frac{1}{2}}/\partial t')(t''-t') \\
&+ \tfrac{1}{2}g'^{-\frac{1}{2}}(g'^{\frac{1}{2}})_{,ij}(q''^{i}-q'^{i})(q''^{j}-q'^{j})+\cdots], \quad (6.41)
\end{aligned}
$$

and noting that $g'^{-\frac{1}{2}}(g'^{\frac{1}{2}})_{,i}=\tfrac{1}{2}g'^{jk}g'_{jk,i}$, etc. The resulting more symmetric form for the Van Vleck determinant emphasizes the symmetry relation

$$D(q'',t''|q',t') = (-1)^n D(q',t'|q'',t''), \tag{6.42}$$

which is a necessary consequence of (2.12). A corollary of (6.25) and (6.42) is the conservation law for a packet moving backwards in time:

$$\partial D/\partial t' + \partial(\dot{q}'^{i}D)/\partial q'^{i} = 0. \tag{6.43}$$

## 7. FEYNMAN QUANTIZATION

In this section we adopt an approach to Feynman's theory due to Pauli,[27] which is based on Van Vleck's work.[25] We introduce the following structure,

$$
\begin{aligned}
\langle q'',t''|q',t'\rangle_c = (2\pi i\hbar)^{-\frac{1}{2}n}g''^{-\frac{1}{4}}D^{\frac{1}{2}}(q'',t''|q',t')g'^{-\frac{1}{4}} \\
\times \exp[i\hbar^{-1}S(q'',t''|q',t')], \quad (7.1)
\end{aligned}
$$

and then show that it can be used to define the exact

quantum transformation function in the limit $t''\to t'$. Expression (7.1) is an invariant under point transformations and, moreover, satisfies the relation

$$\langle q'',t''|q',t'\rangle_c^* = \langle q',t'|q'',t''\rangle_c \tag{7.2}$$

in virtue of (2.12) and (6.42). Next we show that

$$\lim_{t''\to t'} \langle q'',t''|q',t'\rangle_c = \delta(q'',q',t'). \tag{7.3}$$

To do this we first compare the action function $S(q'',t''|q',t')$ with the action function $S_0(q'',t''|q',t')$ for the same system with $a_i$ and $v$ set equal to zero and $g_{ij}$ rendered time-independent. The expansion of $S_0(q'',t''|q',t')$ involves just the portion contained in the curly brackets on the right-hand side of (6.18). Therefore

$$
\begin{aligned}
S(q'',t''|q',t') = S_0(q'',t''|q',t') \\
+ o(q''-q') + o(t''-t'), \quad (7.4)
\end{aligned}
$$

$$D(q'',t''|q',t') = D_0(q'',t''|q',t')[1+o(t''-t')]. \tag{7.5}$$

Moreover, since the Hamiltonian function $H_0=\tfrac{1}{2}g^{ij}p_{0i}p_{0j}$ is a constant of the motion for the modified system,

$$S_0(q'',t''|q',t') = \tfrac{1}{2}(t''-t')g'^{ij}p'_{0i}p'_{0j}. \tag{7.6}$$

Therefore, noting that as $t''\to t'$ the $p'_{0i}$ become infinite except when $q''^{i}=q'^{i}$ (for all $i$), we may write, for an arbitrary function $f$,

$$
\lim_{t''\to t'} \int d_{t''}q''f(q'')\langle q'',t''|q',t'\rangle_c
$$

$$
= \lim_{t''\to t'}(2\pi i\hbar)^{-\frac{1}{2}n}\int dp'_{01}\cdots dp'_{0n}f(q'')g''^{\frac{1}{4}}
$$

$$
\times D_0^{-\frac{1}{2}}(q'',t''|q',t')g'^{-\frac{1}{4}}[1+o(q''-q')+o(t''-t')]
$$

$$
\times \exp[i\hbar^{-1}S_0(q'',t''|q',t')]
$$

$$
= [(t''-t')/2\pi i\hbar]^{\frac{1}{2}n}f(q')g'^{\frac{1}{2}}
$$

$$
\times \int \exp[\tfrac{1}{2}i\hbar^{-1}(t''-t')g'^{ij}p'_{0i}p'_{0j}]
$$

$$
\times dp'_{01}\cdots dp'_{0n}
$$

$$
= f(q'), \tag{7.7}
$$

from which (7.3) follows.

The next step in the identification of $\langle q'',t''|q',t'\rangle_c$ is to show that it nearly satisfies a Schrödinger equation. Using (6.16), (6.25), and (6.38), one finds

$$
\begin{aligned}
i\hbar\langle q'',t''|q',t'\rangle_{c,t''} &- H_{q''}(t'')\langle q'',t''|q',t'\rangle_c \\
&= \tfrac{1}{2}\hbar^2 g''^{-\frac{1}{4}}D^{-\frac{1}{2}}\partial[g''^{\frac{1}{2}}g''^{ij}\partial(g''^{-\frac{1}{4}}D)/\partial q''^{j}]/\partial q''^{i} \\
&\hspace{3cm}\times \langle g'',t''|q',t'\rangle_c \\
&= [\tfrac{1}{12}\hbar^2 R' + o(q''-q') + o(t''-t')]\langle q'',t''|q',t'\rangle_c, \quad (7.8)
\end{aligned}
$$

---

[26] This may be verified by direct computation for a spherical surface. In defining the Riemann tensor there are nearly as many conventions as authors. Expression (6.39) is, for example, the negative of the tensor defined by Bergmann [P. G. Bergmann, *Introduction to the Theory of Relativity* (Prentice-Hall, Inc., New York, 1946), Eq. (11.39)].

[27] W. Pauli, *Feldquantisierung*, lecture notes, Zürich (1950–1951), appendix.

where the operator $H_{q''}(t'')$ is defined by

$$H_{q''}(t'')\psi \equiv -\tfrac{1}{2}\hbar^2 g''^{-\frac{1}{2}}\frac{\partial}{\partial q''^i}\left(g''^{\frac{1}{2}}g''^{ij}\frac{\partial\psi}{\partial q''^j}\right)+i\hbar a''^i\frac{\partial\psi}{\partial q''^i}$$

$$+\left[\tfrac{1}{2}i\hbar g''^{-\frac{1}{2}}\frac{\partial}{\partial q''^i}(g''^{\frac{1}{2}}a''^i)+\tfrac{1}{2}a''^i a''_i+v''\right]\psi, \quad (7.9)$$

when acting on an arbitrary wave function $\psi(q'',t'')$. With the help of (5.31), which can be rewritten in the form

$$(g^{\frac{1}{2}}p_i g^{-\frac{1}{2}})_{q'} = -i\hbar\partial/\partial q'^i, \quad (7.10)$$

one sees that $H_{q''}(t'')$ is the differential form of the operator

$$H \equiv \tfrac{1}{2}g^{-\frac{1}{4}}(p_i-a_i)g^{\frac{1}{2}}g^{ij}(p_j-a_j)g^{-\frac{1}{4}}+v. \quad (7.11)$$

If it were not for the term on the right-hand side of (7.8) this operator could immediately be identified as the quantum analog of the Hamiltonian function (6.15) for the system (6.1). Because of this term, however, the quantum theory that one arrives at by applying the Correspondence Principle via (7.1) is determined *not* by the operator $H$ but by the operator

$$H_+ \equiv H + \tfrac{1}{12}\hbar^2 R. \quad (7.12)$$

That is, in virtue of (7.3) and (7.8), one has

$$\lim_{t''\to t'}(t''-t')^{-1}[\langle q'',t''|q',t'\rangle_c - \langle q'',t''|q',t'\rangle_+]$$

$$= \lim_{t''\to t'}\frac{\partial}{\partial t''}[\langle q'',t''|q',t'\rangle_c - \langle q'',t''|q',t'\rangle_+]=0, \quad (7.13)$$

and hence

$$\langle q'',t''|q',t'\rangle_c = \langle q'',t''|q',t'\rangle_+ + o(t''-t')^2, \quad (7.14)$$

where $\langle q'',t''|q',t'\rangle_+$ is the transformation function generated by the Hamiltonian operator $H_+$. We shall discuss this curious result in further detail after developing the rest of the theory.

Let us first point out that the Schrödinger equation

$$i\hbar\psi_{,t'}(q',t') = H_{+q'}(t')\psi(q',t') \quad (7.15)$$

is invariant under point transformations. This is obvious if the point transformation is time independent, since the right-hand side of (7.9) involves only covariant derivatives and invariant combinations, and the extra term $\tfrac{1}{12}\hbar^2 R'$ in (7.15) is an invariant by itself. However, the conservative time derivative on the left of (7.15) is not invariant under time *dependent* point transformations $q^i=q^i(\bar{q},t)$. From (5.60) one has

$$\psi_{,t}(q,t) \equiv \left(\frac{\partial\psi}{\partial t}\right)_q + \frac{1}{4}\left(\frac{\partial\ln g}{\partial t}\right)_q\psi$$
$$\psi_{,t}(\bar{q},t) \equiv \left(\frac{\partial\psi}{\partial t}\right)_{\bar{q}} + \frac{1}{4}\left(\frac{\partial\ln\bar{g}}{\partial t}\right)_{\bar{q}}\psi \quad \Bigg\}. \quad (7.16)$$

Therefore, from the relation

$$\left(\frac{\partial\psi}{\partial t}\right)_{\bar{q}} = \left(\frac{\partial\psi}{\partial t}\right)_q + \frac{\partial\psi}{\partial q^i}\frac{\partial q^i}{\partial t}, \quad (7.17)$$

together with the transformation law (5.40) for $\ln g$, one may conclude that

$$\psi_{,t}(\bar{q},t) = \psi_{,t}(q,t) + \psi_{,i}\frac{\partial q^i}{\partial t}$$

$$+\frac{1}{4}\left[(\ln g)_{,i}\frac{\partial q^i}{\partial t}+2\frac{\partial\bar{q}^j}{\partial q^i}\frac{\partial^2 q^i}{\partial\bar{q}^j\partial t}\right]\psi. \quad (7.18)$$

The Schrödinger equation (7.15) nevertheless remains invariant, since, as one may readily verify, the transformation laws (6.4) and (6.5) for $a_i$ and $v$ add identical extra terms onto its right-hand side.

The Feynman formulation of the quantum theory follows from (7.14). If the transformation function is broken up into infinitely many pieces by means of the composition law

$$\langle q'',t''|q',t'\rangle_+$$

$$= \int \langle q'',t''|q''',t'''\rangle_+ d_{t'''}q'''\langle q''',t'''|q',t'\rangle_+, \quad (7.19)$$

one may replace $\langle\ \rangle_+$ by $\langle\ \rangle_c$ in each of the pieces and write

$$\langle q'',t''|q',t'\rangle_+ = \lim_{N\to\infty,\Delta t\to 0}\int d_{t^{(1)}}q^{(1)}\cdots$$

$$\times\int d_{t^{(N)}}q^{(N)}\langle q'',t''|q^{(N)},t^{(N)}\rangle_c\cdots$$

$$\times\langle q^{(2)},t^{(2)}|q^{(1)},t^{(1)}\rangle_c\langle q^{(1)},t^{(1)}|q',t'\rangle_c, \quad (7.20)$$

where $\Delta t = \max(t''-t^{(N)}, \cdots t^{(2)}-t^{(1)}, t^{(1)}-t')$, with $t''>t^{(N)}>\cdots>t^{(2)}>t^{(1)}>t'$. From the expression (7.1) for $\langle q'',t''|q',t'\rangle_c$ and the form of the expansion (6.18) for the action, the (in the limit) infinitely multiple integral receives significant contributions from the integrand only when the differences $q''^i-q^{(N)i}$, $\cdots q^{(2)i}-q^{(1)i}$, $q^{(1)i}-q'^i$ are of the order of $(\hbar\Delta t)^{\frac{1}{2}}$ or smaller. Therefore, introducing the symbol $\doteq$ to denote equivalence as far as use in the infinitely multiple integral is concerned, and using the easily verified relation

$$[2\pi i\hbar(t''-t')]^{-\frac{1}{2}n}\int d_{t''}q''f(q'')(q''^i-q'^i)(q''^j-q'^j)$$

$$\times\exp[i\hbar^{-1}S(q'',t''|q',t')]$$

$$= i\hbar(t''-t')g'^{ij}f(q')+o(t''-t')^{\frac{3}{2}}, \quad (7.21)$$

one may write

$$\langle q'',t''|q',t'\rangle_c$$

$$\doteq [2\pi i\hbar(t''-t')]^{-\frac{1}{2}n}[1+\tfrac{1}{12}R'_{ij}(q''^i-q'^i)(q''^j-q'^j)]$$
$$\times \exp[i\hbar^{-1}S(q'',t''|q',t')]$$

$$\doteq [2\pi i\hbar(t''-t')]^{-\frac{1}{2}n}[1+\tfrac{1}{12}i\hbar R'(t''-t')]$$
$$\times \exp[i\hbar^{-1}S(q'',t''|q',t')]$$

$$\doteq [2\pi i\hbar(t''-t')]^{-\frac{1}{2}n}\exp[i\hbar^{-1}S_-(q'',t''|q',t')], \quad (7.22)$$

where $S_-$ is the action function for a "classical" system with Hamiltonian function $H_-\equiv H-\tfrac{1}{12}\hbar^2 R$ and Lagrangian function $L_-\equiv L+\tfrac{1}{12}\hbar^2 R$:

$$S_-(q'',t''|q',t')=S(q'',t''|q',t')+\tfrac{1}{12}\hbar^2 R'(t''-t')$$
$$+o[(t''-t')(q''-q')]. \quad (7.23)$$

The Feynman formulation now becomes

$$\langle q'',t''|q',t'\rangle_+$$

$$=\int_{q',t'}^{q'',t''}\exp\left[i\hbar^{-1}\int_{t'}^{t''}L_-(q,\dot q,t)dt\right]\delta[q], \quad (7.24)$$

where the symbols on the right-hand side are to be understood merely as formal abbreviations:

$$\int_{q',t'}^{q'',t''}\delta[q]$$

$$\equiv \lim_{N\to\infty,\Delta t\to 0}\int\cdots\int[2\pi i\hbar(t''-t^{(N)})]^{-\frac{1}{2}n}d_t{}^{(N)}q^{(N)}\cdots$$

$$\times [2\pi i\hbar(t^{(2)}-t^{(1)})]^{-\frac{1}{2}n}$$

$$\times d_t{}^{(1)}q^{(1)}[2\pi i\hbar(t^{(1)}-t')]^{-\frac{1}{2}n}, \quad (7.25)$$

$$\int_{t'}^{t''}L_-(q,\dot q,t)dt$$

$$\equiv \lim_{N\to\infty,\Delta t\to 0}[S_-(q'',t''|q^{(N)},t^{(N)})+\cdots$$

$$+S_-(q^{(2)},t^{(2)}|q^{(1)},t^{(1)})+S_-(q^{(1)},t^{(1)}|q',t')]. \quad (7.26)$$

The formal "functional integration" indicated in (7.24) has been described by Feynman[3] as a "path summation." According to his interpretation the transformation function $\langle q'',t''|q',t'\rangle_+$ is to be obtained by summing a complex amplitude over all possible paths in $q$, $t$ space between the points $q'$, $t'$ and $q''$, $t''$. The phase of the amplitude associated with each path is obtained by integrating the classical Lagrangian along this path. In the case of systems for which the equations of motion are *linear* it is found that the specification of the path by means of intermediate points $q^{(1)}, t^{(1)}\cdots q^{(N)}, t^{(N)}$, together with the requirement that

the path follow a true classical trajectory between these points [as implied by (7.26)] is actually unnecessary. The functional integral can be evaluated purely formally, without regard to its rigorous definition as an infinitely multiple integral. The result generally contains an unknown (infinite) normalization factor, which is properly accounted for when (7.25) is used but which always cancels out in the computation of any physically measurable quantity. The situation will certainly not be so simple in the general nonlinear cases involving curved spaces, because of the occurrence of a variable metric density in the volume elements $d_t{}^{(1)}q^{(1)}\cdots d_t{}^{(N)}q^{(N)}$.

The result expressed by (7.24) is even more curious than the previous result following from (7.8). In order to obtain the transformation function for a quantized system having Hamiltonian operator $H_+$ one must use, in the Feynman summation, the action corresponding to a classical system having Hamiltonian $H_-$. Whereas Pauli's formalism makes use of the Lagrangian $L$, Feynman must employ $L_-$ to get the same result. When the author first discovered this phenomenon he thought that he had made an error in sign [e.g., in (7.21)] and that the occurrences of $\tfrac{1}{12}\hbar^2 R$ actually cancel each other when one passes from Pauli's formalism on to that of Feynman. A straightforward computation patterned directly after Feynman's original paper,[3] however, demonstrates the reality of the phenomenon.[28]

Instead of stating the result in a symmetric manner one may also state it in the following forms: If the Lagrangian $L$ is used in the Feynman summation then one obtains the transformation function $\langle q'',t''|q',t'\rangle_{++}$ generated by the Hamiltonian operator $H_{++}\equiv H+\tfrac{1}{6}\hbar^2 R$. On the other hand, in order to obtain the transformation function $\langle q'',t''|q',t'\rangle$ generated by the operator $H$ one must use the Lagrangian $L_{--}\equiv L+\tfrac{1}{6}\hbar^2 R$ (corresponding to the Hamiltonian $H_{--}\equiv H-\tfrac{1}{6}\hbar^2 R$) in the Feynman summation. If $q$ space is flat then, of course, all these alternatives coalesce into a single theory. However, in the general case with nonvanishing $R$ there is clearly an ambiguity in making the traditional passage from the classical theory to the quantum theory. The scalar curvature $R$ is constructed out of quantities which already exist in the classical theory, and it has just the right dimensions, when multiplied by $\hbar^2$, to stand as a separate term in the Hamiltonian operator. The choice of a numerical factor to stand in front of $\hbar^2 R$ is undetermined; all choices lead to the same classical theory in the limit $\hbar\to 0$. This, however, is the only ambiguity in the quantum Hamiltonian.

That the quantum theory goes over to the classical theory in the limit $\hbar\to 0$ is particularly transparent in the Feynman formalism. Thus, for example, in (7.24) when $\hbar$ is small the only paths which make in-phase

[28] J. L. Anderson (private communication).

contributions to the formal sum are those which cluster about that path between $q'$, $t'$ and $q''$, $t''$ which makes the action integral stationary, i.e., the classical trajectory. A wave packet $|\psi(q'',t'')|^2$ must move along such a trajectory, the particular trajectory taken depending on phase relationships in the initial wave function $\psi(q',t')$. The Pauli formalism also makes this obvious, for one may write $|\langle q'',t''|q',t'\rangle|^2 \approx |\langle q'',t''|q',t'\rangle_c|^2 = (2\pi\hbar)^{-n}g''^{-\frac{1}{2}}D(q'',t''|q',t')g'^{-\frac{1}{2}}$, and, in virtue of (6.25), this structure satisfies the classical packet conservation law (6.27), which in the quantum theory is simply the law of conservation of probability. This particular structure corresponds to an "exploding" packet, which initially has a delta-function form, with all values of momentum equally probable. However, as Van Vleck's work shows,[25] there is no need to make the initial specification in terms of coordinates $q'^i$; any complete set of commuting variables will do as well, and hence any type of packet may be specified.

The Feynman formalism provides a compact representation not only of the transformation function itself, but also of the matrix elements of arbitrary operators. For example, let $f$ be an arbitrary function of the $q$'s and $t$. Then, adopting the choice $H_{++}$ for the Hamiltonian operator, which results from the use of the simple Lagrangian $L$ in the path summation, we may write

$$\langle q'',t''|f(q(t'''),t''')|q',t'\rangle_{++}$$

$$= \int d_{t'''}q'''\langle q'',t''|q''',t'''\rangle_{++}f(q''',t''')\langle q''',t'''|q',t'\rangle_{++}$$

$$= \int_{q',t'}^{q'',t''} f(q(t'''),t''')$$

$$\times \exp\left[i\hbar^{-1}\int_{t'}^{t''} L(q,\dot{q},t)dt\right]\delta[q]. \quad (7.27)$$

Here it is to be understood that $q'''$, $t'''$ is included among the variable points used to specify the path:

$$\int_{q',t'}^{q'',t''} \delta[q]$$

$$\equiv \lim_{M,N\to\infty,\Delta t\to 0} \int \cdots \int [2\pi i\hbar(t''-t^{(M+N)})]^{-\frac{1}{2}n}$$

$$\times d_{t^{(M+N)}}q^{(M+N)} \cdots [2\pi i\hbar(t^{(M+1)}-t''')]^{-\frac{1}{2}n}$$

$$\times d_{t'''}q'''[2\pi i\hbar(t'''-t^{(M)})]^{-\frac{1}{2}n} \cdots$$

$$\times d_{t^{(1)}}q^{(1)}[2\pi i\hbar(t^{(1)}-t')]^{-\frac{1}{2}n}. \quad (7.28)$$

Matrix elements involving the momentum may be obtained in a similar manner. For example,

$$\langle q'',t''|\tfrac{1}{2}\{f(q(t'''),t'''),p_i(t''')\}|q',t'\rangle_{++}$$

$$= \frac{1}{2}\int d_{t'''}q'''[\langle q'',t''|p_i(t''')|q''',t'''\rangle_{++}$$

$$\times f(q''',t''')\langle q''',t'''|q',t'\rangle_{++} + \langle q'',t''|q''',t'''\rangle_{++}$$

$$\times f(q''',t''')\langle q''',t'''|p_i(t''')|q',t'\rangle_{++}]$$

$$= \frac{1}{2}\int_{q',t'}^{q'',t''} f(q(t'''),t''')[\overleftarrow{p}_i(t''')+\overrightarrow{p}_i(t''')]$$

$$\times \exp\left[i\hbar^{-1}\int_{t'}^{t''} L(q,\dot{q},t)dt\right]\delta[q]. \quad (7.29)$$

Here one makes use of the coordinate representation (5.27) of the momentum operator, and the identity (5.13). The significance of the arrows in the final expression is obvious. The momentum at the point $q'''$, $t'''$ may be defined either with respect to the trajectory coming from the past or with respect to the trajectory going into the future:

$$\overleftarrow{p}'''_i = -\partial S(q^{(M+1)},t^{(M+1)}|q''',t''')/\partial q'''^i, \quad (7.30)$$

$$\overrightarrow{p}'''_i = \partial S(q''',t'''|q^{(M)},t^{(M)})/\partial q'''^i. \quad (7.31)$$

To obtain the symmetrized form involving the anticommutator, one must average the two.

A final example, in which the momenta appear quadratically, is given by

$$\langle q'',t''|g^{-\frac{1}{4}}(t''')p_i(t''')g^{\frac{1}{2}}(t''')f^{ij}(t''')p_j(t''')g^{-\frac{1}{4}}(t''')|q',t'\rangle_{++}$$

$$= -\hbar^2\int d_{t'''}q'''\langle q'',t''|q''',t'''\rangle_{++}$$

$$\times (f'''^{ij}\langle q''',t'''|q',t'\rangle_{++.j})_{.i}$$

$$= \hbar^2\int d_{t'''}q'''f'''^{ij}\langle q'',t''|q''',t'''\rangle_{++.i}\langle q''',t'''|q',t'\rangle_{++.j}$$

$$= \int_{q',t'}^{q'',t''} \overleftarrow{p}_i(t''')f^{ij}(q(t'''),t''')\overrightarrow{p}_j(t''')$$

$$\times \exp\left[i\hbar^{-1}\int_{t'}^{t''} L(q,\dot{q},t)dt\right]\delta[q]. \quad (7.32)$$

Here a covariant integration by parts has been performed,[29] the dot followed by one or more indexes denoting covariant differentiation with respect to the $q'''^i$.

It is now possible to derive Schwinger's dynamical principle directly from Feynman's formulation. Remembering that Schwinger's theory is valid in precisely those cases in which the functional integrals can be evaluated without regard to their rigorous definitions as

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[29] If one applies these procedures to the product of two or more operators $F(t''')$, $G(t''')\cdots$ which are functions of the canonical variables taken at different times, then one obtains the matrix elements of the *time ordered* product $[F(t''')G(t''')\cdots]_+$ provided the path summation is understood to be carried out only over paths which contain no parts moving backwards in time.

infinitely multiple integrals (and hence in which the distinction between $\vec{p}_i$ and $\vec{p}_i$, for example, is unnecessary), one may, in these cases, write purely formally

$$\delta\langle q'',t'' | q',t'\rangle$$

$$=i\hbar^{-1}\int_{q',t'}^{q'',t''} \left\{\delta\int_{t'}^{t''} L dt \exp\left[i\hbar^{-1}\int_{t'}^{t''} L dt\right]\right\}\delta[q]$$

$$=i\hbar^{-1}\left(q'',t'' \left|\delta\int_{t'}^{t''} L dt\right| q',t'\right), \qquad (7.33)$$

the $L$ in the final expression being the operator Lagrangian.

In the more general case it is possible to write an approximate expression for the well-ordered quantum analog of the classical action function. From (5.66), (7.1), and (7.14), we obtain

$$\mathcal{S}_+(q'',t'' | q',t')$$
$$=S(q'',t'' | q',t')-\tfrac{1}{2}i\hbar \ln[D(q'',t'' | q',t')/(2\pi i\hbar)^n]$$
$$+o[\hbar^2(t''-t')^2]. \qquad (7.34)$$

The well-ordered operator form follows from this by the method indicated in Sec. 5. In the case of a free particle in one dimension we have exactly

$$\mathcal{S}(q(t''),t'' | q(t'),t')$$
$$=\tfrac{1}{2}(t''-t')^{-1}[q^2(t'')-2q(t'')q(t')+q^2(t')]$$
$$+\tfrac{1}{2}i\hbar \ln[2\pi i\hbar(t''-t')]. \qquad (7.35)$$

The variation of this operator is given by

$$\delta\mathcal{S}=(t''-t')^{-1}[q(t'')-q(t')][\delta q(t'')-\delta q(t')]$$
$$-\tfrac{1}{2}(t''-t')^{-2}[q^2(t'')-2q(t'')q(t')+q^2(t')](\delta t''-\delta t')$$
$$+\tfrac{1}{2}i\hbar(t''-t')^{-1}(\delta t''-\delta t'), \qquad (7.36)$$

which, since $[q(t''),q(t')]=-i\hbar(t''-t')$, is the same as the variation of the operator

$$S(t'' | t')=\tfrac{1}{2}(t''-t')^{-1}[q(t'')-q(t')]^2$$

$$=\frac{1}{2}\int_{t'}^{t''} \dot{q}^2(t)dt, \qquad (7.37)$$

when written in the form indicated.