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PATH-INTEGRALS IN DYNAMICS

by

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ABSTRACT

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The Lagrangian formulation of quantum dynamics in terms of path-integrals due to Feynman describes systems for which the Hamiltonian is classical in form and quantization is carried out in terms of commutators rather than anticommutators. The difficulty with the Feynman method is the actual evaluation of the path-integral itself. We give an explicit evaluation for classical wave motion in one dimension. This requires an extension of the Feynman method which was introduced by Tobocman and studied in detail by Davies.

We also discuss the work of Corson on the question of a unified formulation of dynamics.

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1. Introduction

The path-integral approach to quantum mechanics (Feynman 1948) provides an alternative to the formulation based on the Schrödinger equation and the usual commutation rules. It does not, however, describe the Dirac field in which operators satisfy certain anti-commutation laws (Tobocman, 1956).

The difficulty with the Feynman method is the actual evaluation of the path-integral itself. Cases which have been explicitly evaluated are those corresponding to the free particle and to the harmonic oscillator (Davies, 1957). A further example is provided by the path-integral formulation of classical wave motion in one dimension. To discuss this we first of all require an extension of the Feynman method which was introduced by Tobocman (1956) and studied in detail by Davies (1963).

2. Extension of Feynman Method

This extension is based on the Hamiltonian of the system rather than on the Lagrangian. In it the time development of the wave function is given by

$$\psi(q'',T) = \int dq' \, K(q', q'', T) \, \psi(q', 0) \, , \qquad (1)$$

which connects the wave function $\psi(q'',T)$ at time T with the wave function $\psi(q',0)$ at an earlier time. The kernel, or path-integral, $K(q',q'',T)$ is given by

$$K(q',q'',T) = \mathcal{N} \sum_{h} \exp i S_h \quad , \tag{2}$$

where

$$S_h = \int_0^T \{ p\dot{q} - H(p,q) \} \, dt \ . \tag{3}$$

In (3), H is the classical Hamiltonian of the system while the subscript h denotes any history of the system specified by two arbitrary functions of time $q(t)$ and $p(t)$ subject to the restrictions $q(0) = q'$, and $q(T) = q''$. Thus S_h is the classical action for a history h. In (2), $\sum_h$ means a sum over all histories which satisfy the end conditions and not only over the history which is the actual classical path between the end-points. The normalization factor $\mathcal{N}$ is chosen so that

$$K(q',q'',0) = \delta(q'-q'') \quad , \tag{4}$$

where δ is the Dirac delta function.

The equivalence of this approach to the usual one based on the Schrödinger equation

$$H\psi = i\frac{\partial\psi}{\partial t} \tag{5}$$

is readily shown by means of setting up operators in a function space and defining an appropriate inner product. This is now outlined.

3. The Operators p and q .

We suppose that the elements of the function space are $f(q)$, $g(q)$, etc. Then, following Davies (1963), we define an inner product (f, g) as follows :

$$(f,g) = \iint dq'\,dq''\,\bar{f}(q'')\,A(q',q'',T)\,g(q')\,, \tag{6}$$

where

$$A(q',q'',T) = N\sum_{h} exp\; i\int_0^T p\,dq\,, \tag{7}$$

and the histories to be summed over are those specified by giving $q(t)$, $p(t)$ arbitrary values over the range $0 \leq t \leq T$

subject to the restrictions

$$q(0) = q', \qquad q(T) = q''. \tag{8}$$

By the method described in section 5 we evaluate the summation in (7) and find that

$$A(q', q'', T) = \delta(q' - q''), \tag{9}$$

a result independent of T. Hence the inner product (f, g) becomes

$$(f, g) = \iint dq'\, dq''\, \bar{f}(q'')\, \delta(q' - q'')\, g(q')$$

$$= \int dq'\, \bar{f}(q')\, g(q'), \tag{10}$$

which corresponds with the frequently used inner product of function space.

We now define operators corresponding to the variables q, p. First, we define the operator Q corresponding to q by

$$(f, Qg) = \iint dq'\, dq''\, \bar{f}(q'')\, B(q', q'', T)\, g(q'), \tag{11}$$

where

$$B(q',q'';T) = \mathcal{N} \sum_h q_h(t) \exp i\int_0^T p\,dq , \tag{12}$$

where a time t has been associated with Q such that $0<t<T$ and once again the summation has to be carried out over all q-p histories subject to the restrictions

$$q(0) = q' , \quad q(T) = q'' . \tag{13}$$

The evaluation of (12) is carried out by the method described in section 5 and we find that

$$B(q',q'';T) = q'\,\delta(q'-q'') . \tag{14}$$

Hence equation (11) becomes

$$\begin{aligned}(f,Qg) &= \iint dq'dq''\,\bar{f}(q'')\,q'\,\delta(q'-q'')\,g(q') \\ &= \int dq'\,\bar{f}(q')\,q'\,g(q') ,\end{aligned} \tag{15}$$

which is identical to the usual representation of the operator corresponding to q .

In a similar way, the operator corresponding to p is defined by

$$(f, Pg) = \iint dq' dq'' \bar{f}(q'') \; C(q', q'', T) \; g(q'), \qquad (16)$$

where

$$C(q', q'', T) = \mathcal{N} \sum_h p_h(t) \; \exp i \int_0^T p \, dq \, . \qquad (17)$$

It can be readily shown that

$$C(q', q'', T) = -i \, \delta'(q'' - q') \, , \qquad (18)$$

where δ' is the first derivative of the Dirac delta function. Hence equation (16) becomes

$$\begin{aligned}
(f, Pg) &= \iint dq' dq'' \, \bar{f}(q'') \, (-i) \, \delta'(q'' - q') \, g(q') \\
&= \int dq'' \, \bar{f}(q'') \int dq' \left\{ i \frac{d}{dq'} \, \delta(q'' - q') \right\} g(q') \\
&= \int dq'' \, \bar{f}(q'') \int dq' \, \delta(q'' - q') \left(-i \frac{dg}{dq'} \right) \\
&= \int dq' \, \bar{f}(q') \left(-i \frac{d}{dq'} \right) g(q') \, , \qquad (19)
\end{aligned}$$

where (19) has been obtained by integration by parts. Equation (19) shows the usual quantum mechanical correspondence of the variable p with the operator $-i\, d/dq$.

4. Equivalence of the path-integral method with the Schrödinger Approach.

Since we have now defined the operators Q, P corresponding to the variables q, p, we can define similarly operators corresponding to q^2 and to p^2 and, indeed, to a function $F(q,p)$. Thus, we write

$$(f, F(Q,P)\, g) = \iint dq'\, dq''\, \bar{f}(q'')\, I(q', q''; T)\, g(q'), \qquad (20)$$

where

$$I(q', q''; T) = N \sum_h F(q_h(t), p_h(t)) \exp i \int_0^T p\, dq. \qquad (21)$$

In the same way we can define the operator

$$\exp\left\{ -i \int_0^T F(Q, P, t)\, dt \right\}$$

by

$$\left(f, \exp\left\{-i\int_0^T F(Q,P,t)\,dt\right\} g\right) = \iint dq'\,dq''\,\bar{f}(q'')\,J(q',q'';T)\,g(q'), \quad (22)$$

where

$$J(q',q'';T) = \mathcal{N}\sum_h \exp i\left(\int_0^T p\,dq - F(q,p,t)\,dt\right). \quad (23)$$

We now choose $F(q,p,t)$ to be equal to $H(q,p,t)$, the Hamiltonian of a system. But now, for this particular choice of $F(q,p,t)$, the kernel J of equation (23) is identical with the kernel K of equations (1), (2) and (3) which determined a function $\psi(q'',T)$ from a function $\psi(q',0)$. So if we write $g(q) = \psi(q,0)$, we have

$$\left(f, \exp\left\{-i\int_0^T H(Q,P,t)\,dt\right\} \psi(q,0)\right) = \int dq''\,\bar{f}(q'')\,\psi(q'',T)$$

$$= \left(f, \psi(q,T)\right), \quad (24)$$

and therefore we have

$$\psi(q,T) = \exp\left\{-i\int_0^T H\,dt\right\} \psi(q,0), \quad (25)$$

which is just the integral form of the Schrödinger equation

$$H\psi = i\frac{\partial\psi}{\partial t} .$$

The equivalence of the path-integral method with the Schrödinger approach is therefore established.

5. Classical Wave Motion

We take the classical wave equation in one space dimension

$$\frac{\partial^2\varphi}{\partial q^2} = \frac{\partial^2\varphi}{\partial t^2} \tag{26}$$

and write it in the two-component form

$$M\psi = i\frac{\partial\psi}{\partial t} , \tag{27}$$

where

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix} , \quad u = \frac{\partial\varphi}{\partial q} , \quad v = \frac{\partial\varphi}{\partial t} , \tag{28}$$

and

$$M = -\sigma P , \tag{29}$$

with

$$\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad P = -i\frac{\partial}{\partial q} . \tag{30}$$

Equation (27) is of Schrödinger type and the equivalence outlined in Section 4 enables us therefore to reformulate (27) as

$$\psi(q'',T) = \int dq' \, K(q',q'',T) \, \psi(q',0) , \tag{31}$$

with

$$K(q',q'',T) = \mathcal{N} \sum_{h} \exp iS_h , \tag{32}$$

and

$$S_h = \int_0^T \{ p\,dq - M\,dt \} . \tag{33}$$

Following Davies (1963) we use a Riemann definition of the integral and write (33) as

$$S_h = \sum_{r=1}^{n} \{ p_r(q_r - q_{r-1}) + \sigma p_r(t_r - t_{r-1}) \} , \tag{34}$$

where a partition $t_0 = 0$, t_1 , t_2 , . . . , $t_n = T$ has been made of the interval and where $q_r = q(t_r)$ and $p_r = p(\tau_r)$ with $t_{r-1} \leq \tau_r < t_r$, and

$$q_0 = q' \, , \quad q_n = q'' \, . \tag{35}$$

Then

$$\exp iS_h = \prod_{r=1}^{n} \exp i \{ p_r (q_r - q_{r-1}) + \sigma p_r (t_r - t_{r-1}) \}$$

$$= \prod_{r=1}^{n} \exp \{ i p_r (q_r - q_{r-1}) \} \{ \cos p_r (t_r - t_{r-1}) + i \sigma \sin p_r (t_r - t_{r-1}) \} . \tag{36}$$

Averaging over the momentum variables p_1 , p_2 , . . . , p_n we obtain

$$\int_{-\infty}^{\infty} dp_1 \cdots \int_{-\infty}^{\infty} dp_n \exp i S_h = \prod_{r=1}^{n} \int_{-\infty}^{\infty} dp_r \exp \{ i p_r (q_r - q_{r-1}) \}$$

$$\times \{ \cos p_r (t_r - t_{r-1}) + i \sigma \sin p_r (t_r - t_{r-1}) \}$$

$$= \prod_{r=1}^{n} \{ \pi (I + \sigma) \, \delta (q_r - q_{r-1} + t_r - t_{r-1})$$

$$+ \pi (I - \sigma) \, \delta (q_r - q_{r-1} - t_r + t_{r-1}) \} , \tag{37}$$

where I is the unit 2×2 matrix, and where we have used the result

$$\int_{-\infty}^{\infty} dp \exp ipq = 2\pi\delta(q) . \tag{38}$$

The summation over histories is now obtained by integration over $q_1, q_2, \ldots, q_{n-1}$, so that

$$\sum_h \exp iS_h = \int_{-\infty}^{\infty} dq_1 \cdots \int_{-\infty}^{\infty} dq_{n-1} \prod_{r=1}^{n} \{\pi(I+\sigma)\,\delta(q_r - q_{r-1} + t_r - t_{r-1}) + \pi(I-\sigma)\,\delta(q_r - q_{r-1} - t_r + t_{r-1})\}. \tag{39}$$

Performing the integration over q_1 we get

$$\int_{-\infty}^{\infty} dq_1 \{\pi(I+\sigma)\,\delta(q_1 - q_0 + t_1 - t_0) + \pi(I-\sigma)\,\delta(q_1 - q_0 - t_1 + t_0)\}$$
$$\times \{\pi(I+\sigma)\,\delta(q_2 - q_1 + t_2 - t_1) + \pi(I-\sigma)\,\delta(q_2 - q_1 - t_2 + t_1)\}$$

$$= \pi^2(I+\sigma)^2\,\delta(q_2 - q_0 + t_2 - t_0) + \pi^2(I-\sigma)^2\,\delta(q_2 - q_0 - t_2 + t_0), \tag{40}$$

since

$$(I+\sigma)(I-\sigma) = 0 , \tag{41}$$

and

$$\int_{-\infty}^{\infty} dq_1 \, \delta(q_1+a) \, \delta(b-q_1) = \delta(a+b) . \tag{42}$$

The integrals over $q_2, q_3, \ldots, q_{n-1}$ can be evaluated in the same way and we obtain

$$\sum_h \exp i S_h = \pi^n (I+\sigma)^n \delta(q''-q'+T) + \pi^n (I-\sigma)^n \delta(q''-q'-T). \tag{43}$$

Using the relations

$$(I \pm \sigma)^n = 2^{n-1} (I \pm \sigma) , \tag{44}$$

and introducing the normalization factor $\mathcal{N} = (2\pi)^{-n}$, we have

$$K(q',q'',T) = \tfrac{1}{2} (I+\sigma) \, \delta(q''-q'+T) + \tfrac{1}{2} (I-\sigma) \, \delta(q''-q'-T) . \tag{45}$$

Equations (31) and (45) together provide a path-integral formulation of classical wave motion. With given initial conditions, equation (31) has a solution which agrees of course with the standard D'Alembert solution.

6. Unified formulation of dynamics

We now consider the work of Corson (1963) on the question of finding a single postulate (if one exists) that would cover both classical and quantum dynamics. This postulate, therefore, must lead to the Schrödinger equation in the quantum case and to Lagrange's equations (or equivalents) in the classical case.

The classical case is given by

$$\delta S = 0 , \tag{46}$$

where S is the action defined in equation (3). Equation (46) means that S is stationary with respect to a small variation in the path between the endpoints $(q', 0)$ and (q'', T). Now Hamilton's principle (46) is really just the simplest form of a stationary condition involving S. It could be replaced by

$$\delta F(S) = 0 \tag{47}$$

with F some reasonable function of S . Corson's choice of F is

$$F(S) = \exp iS \,, \tag{48}$$

because of the form of the path-integral K in equation (2).

Corson (1963) then postulates

$$\delta \sum_{h} \exp i S_h = 0 \tag{49}$$

as the fundamental equation of dynamics. There are two cases, namely, (i) the definite path case, and (ii) the indefinite path case:

(i) definite path. If there is only <u>one</u> path h , then equation (49) reduces to

$$\delta \exp iS = 0 \,,$$

or

$$\delta S = 0 \,, \tag{50}$$

and equation (50) leads, of course, to Lagrange's equations. This then covers the classical case.

(ii) indefinite path. If there are many paths, $\sum_{h} \exp iS_h$ is a function of the end-points only, and since the end-points remain fixed under the δ -variation, it follows that

$$\delta \sum_{h} \exp iS_h = 0 \tag{51}$$

trivially. This condition therefore does not appear to lead to anything. The classical case $\delta S = 0$ leads to Lagrange's equations, but the many path case does not tell us what function of the end-points $\sum_{h} \exp iS_h$ actually is. This requires an additional postulate - one involving the notion of state or wave function.

Thus the conclusion would seem to be that Corson's single postulate is not enough. To formulate quantum dynamics from classical action expressions one must postulate the time evolution of the wave function as Feynman did.

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