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# The Feynman–Kac Formula and the Hamilton–Jacobi Equation

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By means of a theory of representations of canonical transformations we establish a connection between the Feynman–Kac formula and the Hamilton–Jacobi equation. 

## I. INTRODUCTION

In this work we present a derivation of the Feynman–Kac formula based on a theory of nonunitary representations of canonical transformations. The basic idea is that the flow in $\mathbb{R}^{2n}$ of a mechanical system with Hamiltonian

$$H(q, p) = K(p) + V(q) \tag{I.1}$$

is mapped to a semigroup of operators, on functions on $\mathbb{R}^n$, having infinitesimal generator

$$G = K(-\nabla) + V(q), \tag{I.2}$$

where assume $K$ to be real analytic and $V$ to be smooth.

To construct the mapping that will do this we must recall how to desribed time evolution in classical mechanics by means of canonical transformations, and then we must introduce a class of non-unitary representations of this group of canonical transformations.

For the sake of completeness we will recall a few of the basics from classical mechanics. The reader can refer to [1] or [11] for more details.

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The time evolution of the system is described by the (Hamiltonian) set of equations

$$\dot{q}_i = \partial H/\partial p_i, \qquad \dot{p}_i = -\partial H/\partial q_i, \qquad i = 1, 2, \ldots, n \tag{I.3}$$

plus initial conditions. We shall assume that a global solution to (I.3) exists through every point $(q, p)$ in $\mathbb{R}^{2n}$.

We shall say that a function $F(q, p, t)$ generates the canonical transformation $(q, p) \to (Q, P)$ whenever the transformation equations

$$Q_i = \partial F/\partial P_i, \qquad p_i = \partial F/\partial q_i, \qquad i = 1, 2, \ldots, n \tag{I.4}$$

can be globally solved for $(Q, P)$ in terms of $(q, p)$ and vice versa.

Two basic examples, sufficient for our need, correspond to the cases

$$F(q, P, t) = P \cdot \phi(q) + h(q, t) \tag{I.5a}$$

$$F(q, P, t) = q \cdot \psi(P) + g(P, t), \tag{I.5b}$$

where $A \cdot B$ stands for the euclidean scalar product in $\mathbb{R}^n$, and $\phi$, $\psi$ denote two smootly invertible functions on $\mathbb{R}^n$ (which may depend on $t$, in which case we assume joint smoothness in all variables and invertibility for each $t$). Also $h$ and $g$ are assumed smooth in all variables. Since canonical transformations are changes of variables, and as such can be composed, we expect such a composition to be reflected at the level of their generating functions. This is the content of the following lemma which can be rapidly verified for the cases (I.5).

LEMMA I.6. *Let $F_1(q^1, p^1)$ and $F_2(q^2, p^2)$ be the generating functions of the canonical transformations $(q^1, p^1) \to (q^2, p^2)$ and $(q^2, p^2) \to (q^3, p^3)$; then*

$$(F_2 \circ F_1)(q^1, p^3) = F_1(q^1, p^2) - q^2 \cdot p^2 + F_2(q^2, p^3) \equiv F(q^1, p^3) \tag{I.7}$$

*generates the composition $(q^1, p^1) \to (q^3, p^3)$. In* (I.7), *$q^2$ and $p^2$ are to be eliminated with the aid of* (I.4).

*Comments.* (i) The generating functions we deal with are usually described as being of the "second type" and written with a 2 as the subindex. For us subindices denote different generating functions of the second type.

(ii) It is easy to verify that each of the classes (I.5) is a group under the composition in Lemma (I.7). The open question is how big is the group they generate together? In what follows we shall see why they are basic.

LEMMA I.8. *The inverses under the composition introduced in Lemma* (I.7) *of each of the classes* (I.5) *are*

$$\bar{F}(Q, p, t) = p \cdot \phi^{-1}(q) - h(\phi^{-1}(Q), t) \tag{I.9a}$$

$$\bar{F}(Q, p, t) = Q \cdot \psi^{-1}(P) - g(\psi^{-1}(P), t). \tag{I.9b}$$

*Proof.* Verify it.

PROPOSITION I.10. *For a system with Hamiltonian* $H(q, p) = K(p)$, $S(q, P, t) = q \cdot P - K(P)\, t$ *generates the transformation that brings the system to rest, and satisfies*

$$\frac{\partial S}{\partial t} + H(q, \nabla_q S) = 0, \qquad S(q, P, 0) = q \cdot P. \tag{I.11}$$

*Proof.* Easy.

*Comments.* (I.11) is called the Hamilton–Jacobi equation, and $S(q, P, 0) = q \cdot P$ generates the identity transformation. Note as well that it is of the type (I.5b).

We shall proceed to obtain a solution of (I.11) when $H(q, p) = K(p) + V(q)$. For that we need some preliminaries.

Note to begin with that for $H(q, p) = K(p) + V(q)$ the solution to (I.3) up to $O(\varepsilon^2)$ with $|t| < \varepsilon$ is given by

$$q(t) = Q + (\nabla_p K)(P)\, t$$
$$p(t) = P - (\nabla_q B)(Q)\, t$$

for $|t| < \varepsilon$. These can be rewritten up to $O(\varepsilon^2)$ as

$$\begin{aligned} Q &= q - (\nabla_p K)(P)\, t \\ p &= P - (\nabla_q V)(q)\, t, \end{aligned} \tag{I.12}$$

which are the transformation equations determined by the generating function

$$\begin{aligned} &S_\varepsilon(q, P, t) \equiv (F_k \circ F_v)(q, P, t) \equiv q \cdot P - (K(P) + V(q))\, t \\ &F_v(q, P, t) = q \cdot P - V(q)\, t \qquad \text{and} \qquad F_k(q, P, t) = q \cdot P - K(P)\, t. \end{aligned} \tag{I.13}$$

Let us now bring the system from time $t$ to time 0 by a sequence of infinitesimal canonical transformations. For positive $n$ define for $0 \leqslant k \leqslant n$

$$q^k = q\left(t\left(1 - \frac{k}{n}\right)\right), \qquad p^k = p\left(t\left(1 - \frac{k}{n}\right)\right) \tag{I.14}$$

and for $0 \leqslant k \leqslant n$

$$S_k\left(q^k, p^{k+1}, \frac{t}{n}\right) = q^k \cdot p^{k+1} - (K(p^{k+1}) + V(q^k))\frac{t}{n}. \tag{I.15}$$

The relationship between $(q^k, p^k)$ and $(q^{k+1}, p^{k+1})$ is determined by (I.12) via (I.15). Consider now the composition

$$\begin{aligned} &S_{n-1} \circ S_{n-2} \circ \cdots \circ S_1 \circ S_0 \\ &\quad = S_0\left(q^0, p^1, \frac{1}{n}\right) - q^1 \cdot p^1 + S_1\left(q^1, p^2, \frac{t}{n}\right) - \cdots \\ &\quad\quad - q^{n-1} \cdot p^{n-1} + S_{n-1}\left(q^{n-1}, p^n, \frac{t}{n}\right) \\ &\quad = \sum_1^{n-1} p^k \cdot (q^{k-1} - q^k) - \sum_0^{n-1} H(q^k, p^{k+1})\frac{t}{n} + q^{n-1} \cdot p^n \end{aligned} \tag{1.16}$$

and we are ready to state the novel, but expected,

PROPOSITION I.17. *Assuming that the system* (I.3) *has global solutions passing through every point* $(Q, P)$ *in phase space and that* $(q(t), p(t)) = (q(Q, P, t), P(Q, P, t))$ *can be solved for* $(Q, p)$ *in terms of* $(q, P)$ *for* $0 \leqslant t \leqslant T$, *then the Riemann sums* (I.16) *converge to*

$$\lim_{n \to \infty} S_n(q, p^n, t) = S_0(q, p) + \int_0^t \{p(s)\, dq(s) - H(q(s), p(s))\, ds\}, \tag{I.18}$$

*where* $S_0(q, p) = \lim_{n \to \infty} q^{n-1} \cdot p^n = Q \cdot P$ *with* $Q = Q(q, p)$. *Moreover, the solution to* (I.9) *can be represented by the right hand side of* (I.18).

*Proof.* From the comments prior to the statement and the hypothesis the existence of the limits is clear. The second contention of the proposition is known, but we present another proof for completeness. Let $(q(t), p(t))$ be the solution to (I.3) through $(Q, P)$ and put, for $t > 0$, $0 \leqslant s \leqslant t$,

$$(\hat{q}(s), \hat{p}(s)) = (q(t-s), p(t-s)), \qquad \hat{S}(s) = S(\hat{q}(s), P, t-s).$$

Therefore if we prove that $\nabla_q S(q, P, t) = p(t)$, then

$$\frac{d\hat{S}}{ds} = \nabla_q \hat{S} \cdot \hat{q} - \frac{\partial S}{\partial t} = -\hat{p}(t-s)\, \dot{q}(t-s) + H(q(t-s), q(t-s)),$$

and integrating from 0 to $t$ we obtain

$$S(\hat{q}(t), P, 0) - S(\hat{q}(0), P, t = -\int_0^t (p \cdot \dot{q} - H)\, dt.$$

Since $\hat{q}(t) = Q$ and $\hat{q}(0) = q(t)$

$$S(q, P, t) = Q \cdot P + \int_0^t (p \cdot \dot{q} - H(q, p))\, dt,$$

and we can now express $Q$ in terms of $q$, $P$ and $t$. In conclusion note that if we put $\xi_i = \partial S/\partial q_i$, then differentiating (I.11) with respect to $q_i$ and making use of (I.3) we obtain

$$\frac{\partial \xi_i}{\partial t} + \dot{q} \cdot \nabla_q \xi_i - \dot{p}_i = 0, \qquad \xi_i(q, P, 0) = P_i, \qquad i = 1, 2 \cdots$$

or equivalently $d(\xi_i - p_i)/dt = 0$. Since $\xi_i(q, P, 0) = p_i(0) = P_i$ we obtain

$$\xi_i = \frac{\partial S}{\partial q_i}(q, P, t) = p(t)$$

which concludes our proof.

*Comment.* It is now clear why we called the generating functions of the types (I.5a) and (I.5b) basic.

## II. Representation of Canonical Transformations

Here we introduce a non-unitary representation of the class of canonical transformations introduced above which turns out to be an antihomomorphism with respect to the composition law introduced in (I.6). As usual we shall denote by $C_k^\infty$ the class of functions $f\colon \mathbb{R}^n \to \mathbb{R}$ which are infinitely differentiable and have compact support.

Definition (II.1). Let $F(q, P, t)$ be such that $F(q, ik, t)$ makes sense for $k$ in $\mathbb{R}^n$ and $i = \sqrt{-1}$. For $f(Q) \in C_k^\infty$ put

$$(T_F f)(q) = \int e^{-F(q, ik, t)} \hat{f}(k)\, dk/(2\pi)^n, \tag{II.2}$$

where $\hat{f}(k) = \int e^{ik \cdot Q} f(Q)\, dQ$.

We shall drop $t$ for a while.

LEMMA II.3. *For $F(q, P, t) = \psi(q) \cdot P + h(q)$ with $\psi: \mathbb{R}^n \to \mathbb{R}^n$ a diffeomorphism and $h(q)$ in $C^\infty$ we have $T_F: C_K^\infty \to C_K^\infty$ and $T_{F_1} T_{F_2} = T_{F_2 \circ F_1}$ on $C_k^\infty$.*

*Proof.* It suffices to note that $(T_F f)(q) = e^{-h(q)} f(\psi(q))$. Since $\psi$ maps compacts onto compacts, the first assertion follows. The second is even simpler.

LEMMA II.4. *Let $F(q, P, t) = q \cdot P + g(P)$, with $g(P)$ real analytic. Then $T_F: C_k^\infty \to C_k^\infty$ and $T_{F_1} T_{F_2} = T_{F_2 \circ F_1}$ on $C_k^\infty$.*

*Proof.* From the fact that $g$ is analytic we obtain

$$e^{-g(ik)} \hat{f}(ik) = \int (e^{-g(\nabla_Q)} e^{ik \cdot Q})\, f(Q)\, dQ = \int e^{ik \cdot Q} (e^{-g(-\nabla_Q)} f(Q))\, dQ.$$

Since $\exp(-g(\nabla_Q))$ is a local operator, $\exp(-g(\nabla_Q) f))(Q)$ is of compact support whenever $f(Q)$ is so. The rest is easy.

From this and proposition (I.10) we obtain

PROPOSITION II.5. *Let $S(q, P, t) = q \cdot P - H(P)\, t$. Then for $f \in C_k^\infty$, $n(q, t) = (T_{S(t)} f)(q)$ satisfies*

$$\frac{\partial u}{\partial t} = H(-\nabla_q)\, u, \qquad u(q, 0) = g(q). \tag{II.6}$$

*Proof.* Easy.

Observe that in (II.5) or (II.6) there is no restriction upon the sign of $t$. Such restrictions depend on the class of functions we deal with.

The example shown in (II.5), in addition to illustrating the non-unitary representation of transformations of type (I.5b), is the basic example in which ideas of different fields came together. In [2, 12] two approaches to the study of (II.6) appear; in [3] Feinsilver presents a relationship among integrable systems, special polynomials, and probability semigroups.

Some of the probabilistic aspects of the "generalized processes" associated to semigroups like (II.6) are studied in [6–11]. The problem with semigroups associated to solutions to (II.6) is that they cannot be used to provide honest measures on path spaces, but only finitely additive measures (measures on cylinder sets only!).

## III. The Feynman–Kac Formula

Let $(X_t)$ be a Markov process on $\mathbb{R}^n$ with transition operator $P_t$ and (weak) infinitesimal generator $G$. The Feynman–Kac Formula ([4, 5], or [15]) provides us with a probabilistic representation of the solution to

$$\frac{\partial u}{\partial t} = Gu + Vu, \qquad u(q, 0) = f(q) \tag{III.1}$$

in terms of integration on path space. The result is

$$u(q, t) = E^q\left[f(X_t) \exp \int^t V(X_s)\, ds\right], \tag{III.2}$$

where the class of potentials, or source terms, $V(q)$ such that (III.2) makes sense depends on each particular process. (See also [3] for additional versions.)

We now show how (III.2) is derived by using the representation theory and what the problems for its general validity are.

To begin with consider a generalized process, $X_t$ with semigroup $P_t$ and generator $G = K(-\nabla)$. We noted such semigroups in Proposition II.5. By generalized we mean that perhaps the cylindrical measures defined by

$$\begin{aligned} &E^q[f_1(X_{t_1}) \cdots f_n(X_n)\\ &\quad = \int \cdot \int f_1(q_1) \cdots f_n(q_n)\, P_{t_1}(q, dq_1)\, P_{t_2 - t_1}(q_1, dq_2) \cdots P_{t_n - t_{n-1}}(q_{n-1}, dq_n) \end{aligned} \tag{III.3}$$

for $0 \leqslant t_1 \leqslant \cdots \leqslant t_n$ and bounded $f_1, ..., f_n$ cannot be extended to measures on the set of all paths on $\mathbb{R}^n$. Consider now a perturbation $\tilde{G}$ of $G$ given by

$$\tilde{G} = G + V(q) = K(-\nabla) + V(q) \tag{III.4}$$

to which we can associate a mechanical system with Hamiltonian $H(q, p) = K(p) + V(q)$.

We saw in Section I that the Hamilton–Jacobi function $S(q, P, t)$ describing the evolution of such systems can be obtained as the limit of $S^{(n)}(q, P, t)$ where $S^{(n)}(q, P, t) = (S_{n-1} \circ S_{n-2} \circ \cdots \circ S_0)(q, P, t)$ with $S_k(q^k, P^{k+1}, t) = (F_K \circ F_V)\, q^k, P^{k+1}, t/n)$. From Section II we know that

$$(T_V T_K f)(q, \varepsilon) = e^{-V(q)\varepsilon}(P_\varepsilon f)(q) = e^{-V(q)\varepsilon} E^q[f(X_\varepsilon)]$$

and therefore, an application of the simple Markov property yields

$$\left(\prod_{k=0}^{n-1} T_{S_k}\right) f(q, t) = E^q\left[f(X_t) \exp \sum_{k=1}^{n} V\left(X\left(t\frac{k}{n}\right)\right)\right]. \tag{III.5}$$

Nothing very stringent about the function $V(q)$ or the sample paths is needed to ensure the identity $\lim_n \sum_1^n V(X(t(k/n))) = \int_0^t V(X(s))\, ds$. When the measures $E^q(\cdot)$, defined on cylinder sets by III.3, extend to measures on the set of all trajectories on $\mathbb{R}^n$, our version of the product formula is contained in

PROPOSITION III.6. *Assume that $(X_t)$ is a Markov process on $\mathbb{R}^n$ with $t \to X_t$ being almost surely right continuous on $[0, \infty)$ and $V(q)$ being continuous and such that $E^q[\exp \int_0^t V(X(s))\, ds]$ is finite for all $q$ and $t$. Then*

$$\lim_{n \to \infty} \left(\sum_{k=0}^{n-1} T_{S_k}\right) f(q, t) = E^q\left[f(X_t) \exp \int_0^t V(X(s))\, ds\right] \tag{III.7}$$

*for all $f \in C_K^\infty$.*

The stage is set so that the proof of (III.6) is obvious. To conclude we have

PROPOSITION III.8. *Whenever $T_{S(t)}$ is defined and for $u, t \geqslant 0$ $T_{S(t+u)} = T_{S(t)} T_{S(u)}$ we have under the hypotheses of* (III.6)

$$(T_{S(t)} f)(q, t) = E^q\left[f(X_t) \exp \int_0^t V(X(s))\, ds\right]. \tag{III.9}$$

*Proof.* Both sides are semigroups and since

$$\begin{aligned}\frac{\partial}{\partial t}(T_{S(t)} f)(q, t)\Big|_{t=0} &= \int \left\{ -\frac{\partial S}{\partial t}\Big|_{t=0} e^{-S(q, ik, 0)} \hat{f}(k) \right\} dk/(2\pi)^n \\ &= \int [K(ik) + V(q)]\, e^{-ik \cdot q} \hat{f}(k)\, dk/(2\pi)^n = (\tilde{G} f)(q),\end{aligned}$$

since $\partial S/\partial t = -K(\nabla S) + V(q)$ and $S(q, P, 0) = q \cdot P$.

Since both sides are semigroups with the same infinitesimal generator the proof is complete.

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