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LETTER TO THE EDITOR

New path integral representation of the quantum mechanical propagator

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Abstract. A new path integral representation of the quantum mechanical propagator is proposed, which is even more intimately connected with classical mechanics than the Feynman path integral. The emergence of the semiclassical propagator is discussed in detail. It is argued that those paths which actually contribute in the new path integral have a very simple relation with the classical dynamical trajectories in configuration space.

As is well known, the Feynman path integral representation of the quantum mechanical propagator has the form (Feynman and Hibbs 1965, Kleinert 1990, Schulman 1981)

$$\langle x'', t'' | x', t' \rangle = \int \mathscr{D}x(t) \,\delta(x'' - x(t')) \,\delta(x' - x(t')) \exp\{(i/\hbar)S[x(\cdot)]_{t'}^{t''}\} \tag{1}$$

where $S[x(\cdot)]_{t'}^{t''}$ denotes the classical action along a generic path x(t)

$$S[x(\cdot)]_{t'}^{t''} = \int_{t'}^{t''} \mathrm{d}t \, L(x(t), \dot{x}(t), t).$$
⁽²⁾

A large variety of quantum dynamical problems can be successfully handled by this strategy, which is receiving an ever growing interest.

We shall be concerned throughout with the (non-relativistic) Lagrangian

$$L(x, \dot{x}, t) = \frac{1}{2}m\dot{x}_{i}\dot{x}_{i} + \Omega_{i}(x, t)\dot{x}_{i} - \Phi(x, t)$$
(3)

describing a point particle \mathscr{S} (mass *m*, no spin) with configuration space $\mathscr{M} = \mathscr{R}^N$. Still, all considerations presented in this letter can easily be generalized to the case $\mathscr{M} = (\text{Riemann manifold})$ (Defendi and Roncadelli 1992a) as well as to the relativistic counterpart of Lagrangian (3) (Defendi and Roncadelli 1992b).

An important remark often made in connection with equation (1) is that the Feynman path integral provides a very appealing link between classical and quantum dynamics, since the *classical* action *explicitly* appears in equation (1). This circumstance permits a straightforward treatment of the semiclassical approximation via a stationary phase mechanism. Basically, what happens is that as $\hbar \rightarrow 0$ the dominant contribution in (1) comes from paths close to the classical dynamical trajectory $q(t; x', t'; x'', t'') \in \mathcal{M}$ joining (x', t') with (x'', t''). Standard arguments then imply that the semiclassical propagator can be evaluated in a simple manner and reads (Schulman 1981)

$$\langle x'', t''|x', t'\rangle_{\rm SC} = \left(\frac{\mathrm{i}}{2\pi\hbar}\right)^{N/2} \left(\det\left|\frac{\partial^2 S(x'', t''; x', t')}{\partial x'_i \partial x'_j}\right|\right)^{1/2} \exp\left(\frac{\mathrm{i}}{\hbar}S(x'', t''; x', t')\right)$$
(4)

with

$$S(x'', t''; x', t') \equiv S[q(\cdot; x', t'; x'', t'')]_{t'}^{t''}.$$
(5)

Our aim is to point out that an *alternative* path integral representation of the quantum mechanical propagator exists, which is *even more closely related to classical dynamics*. As we are going to show, the *new* path integral representation holds

$$\langle x'', t'' | x', t' \rangle = \exp\left(\frac{i}{\hbar} [S(x'', t'') - S(x', t')]\right) \int \mathscr{D}x(t)\delta(x'' - x(t''))\delta(x' - x(t'))$$
$$\times \exp\left\{\frac{i}{\hbar} \frac{m}{2} \int_{t'}^{t''} dt [\dot{x}_i(t) - \mathscr{V}_i(x(t), t; [S(\cdot)])]^2\right\}$$
(6)

where we have set (for notational simplicity)

$$\mathcal{V}_i(x,t;[S(\cdot)]) = \frac{1}{m} \left(\frac{\partial}{\partial x_i} S(x,t) - \Omega_i(x,t) \right).$$
(7)

We stress that S(x, t) in (6) is an *arbitrary* solution to the classical Hamilton-Jacobi equation associated with Lagrangian (3)

$$\frac{\partial}{\partial t}S(x,t) + \frac{1}{2m} \left(\frac{\partial}{\partial x_i}S(x,t) - \Omega_i(x,t)\right)^2 + \Phi(x,t) = 0.$$
(8)

Notice that the RHS of (6) does not (globally) depend on which specific solution S(x, t) is used (why this is possible will become clear later on). Generally speaking, S(x, t) is expected to be regular only over a certain *finite* time interval T, because of the existence of *focal points* in \mathcal{M} (integrable systems are an exception) (Courant and Hilbert 1962). Accordingly, equation (6) makes sense only under the assumption |t''-t'| < T. This is, however, not a real limitation. One can in fact compute $\langle x'', t'' | x', t' \rangle$ first for |t''-t'| < T using (6). The latter result can next be *trivially* extended to *arbitrary* times thanks to the convolution property

$$\langle x'', t'' | x', t' \rangle = \int_{-\infty}^{+\infty} dx''' \langle x'', t'' | x''', t''' \rangle \langle x''', t''' | x', t' \rangle$$
(9)

since focal points in \mathcal{M} disappear after quantization.

Let us now prove equation (6). We start by rewriting the second square bracket in (6) in a somewhat fancy way

$$\frac{1}{2}m[\dot{x}_{i}(t) - \mathcal{V}_{i}(x(t), t; [S(\cdot)])]^{2}$$

$$= \left[\frac{1}{2}m\dot{x}_{i}(t)\dot{x}_{i}(t) + \Omega_{i}(x(t), t)\dot{x}_{i}(t) - \Phi(x(t), t)\right]$$

$$- \left[\frac{\partial}{\partial t}S(x, t) + \dot{x}_{i}\frac{\partial}{\partial x_{i}}S(x, t)\right]\Big|_{x=x(t)}$$

$$+ \left[\frac{\partial}{\partial t}S(x, t) + \frac{1}{2}m\mathcal{V}_{i}(x, t; [S(\cdot)])\mathcal{V}_{i}(x, t; [S(\cdot)]) + \Phi(x, t)\right]\Big|_{x=x(t)}$$
(10)

which is nothing but an *identity*. We proceed by focusing our attention on the RHS of equation (10). Clearly, the last bracket vanishes because of (7) and (8). Moreover, the first bracket is just Lagrangian (3) and the second one is the total time derivative of S(x, t). Thus, (10) becomes

$$\frac{1}{2}m[\dot{x}_i(t) - \mathcal{V}_i(x(t), t; [S(\cdot)])]^2 = L(x(t), \dot{x}(t), t) - \frac{d}{dt}S(x(t), t).$$
(11)

Finally, we insert (11) into (6). Then the time derivative of S(x(t), t) yields a boundary term which precisely *cancels* the exponential prefactor. So what is left over turns out to *coincide* with the RHs of (1) (on account of (2)). Observe that we have only been assuming that S(x, t) obeys (8), therefore (6) should be true for any such S(x, t). \Box

A question which arises quite naturally is how the semiclassical propagator emerges by taking equation (6) as starting point. As a preliminary step, we recall that once a particular (arbitrary) integral S(x, t) of (8) is known, a family of trajectories in \mathcal{M} is provided by the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}q_i(t) = \mathcal{V}_i(q(t), t; [S(\cdot)]). \tag{12}$$

We denote by $q(t; x', t'; [S(\cdot)])$ the solution to (12) controlled by S(x, t) with initial condition q(t') = x'. Then $q(t; x', t'; [S(\cdot)])$ is just the classical dynamical trajectory of \mathscr{S} in \mathscr{M} selected by the initial data $q(t') = x', p(t') = (\nabla S)(x', t')$ (Arnold 1978). In particular, corresponding to the following solution to (8) (Sudarshan and Mukunda 1974)

$$S(x, t) = S_{*}(x, t) \equiv S(x, t; x'', t'')$$
(13)

we get

$$q(t; x', t'; [S_{*}(\cdot)]) = q(t; x', t'; x'', t'').$$
(14)

We shall stick throughout to the choice $S(x, t) = S_*(x, t)$, working (for simplicity) in one dimension. As usual, we parametrize the paths in (6) as

$$x(t) = q(t; x', t'; [S_{*}(\cdot)]) + y(t)$$
(15)

so y(t') = y(t'') = 0 (we are implicitly assuming |t'' - t'| small enough so as to avoid focal points, hence the parametrization (15) is *unique*). Manifestly, even in the present situation the semiclassical approximation arises from the stationary phase mechanism (as applied to (6)). Standard arguments then entail that the semiclassical propagator is given by

$$\langle x'', t'' | x', t' \rangle_{SC}$$

$$= \exp\left(\frac{\mathrm{i}}{\hbar} S(x'', t''; x', t')\right) \int \mathscr{D}y(t) \delta(y(t')) \delta(y(t'))$$

$$\times \exp\left\{\frac{\mathrm{i}}{\hbar} \frac{m}{2} \int_{t'}^{t'} \mathrm{d}t [\dot{y}_i(t) - \mathscr{V}'(y(t), t; [S_*(\cdot)])]^2\right\}$$

$$(16)$$

where the prime denotes differentiation with respect to x. The path integral in (16) can easily be computed by the *shifting method* (Felsager 1981), which leads to the result

$$\langle x'', t'' | x', t' \rangle_{\rm SC} = \left[\frac{m}{2\pi i \hbar \omega (t'') \int_{t'}^{t''} dt \, \omega(t)^{-2}} \right]^{1/2} \exp\left(\frac{i}{\hbar} S(x'', t''; x', t')\right)$$
(17)

having set

$$\omega(t) = \exp\left\{\int_{t'}^{t''} ds \, \mathcal{V}'(q(s; x', t'; [S_{*}(\cdot)]), s; [S_{*}(\cdot)])\right\}.$$
(18)

We proceed by considering the Jacobi equation (Kleinert 1990, Zinn-Justin 1989)

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$$\left[\frac{d^2}{dt^2} + \frac{1}{m}\Phi''(q(t; x', t'; x'', t''), t)\right]k(t) = 0.$$
(19)

A well known fact about any solution to (19) is that the remarkable relation holds (Zinn-Justin 1989)

$$\frac{m}{k(t'')k(t')\int_{t'}^{t''} dt \, k(t)^{-2}} = -\frac{\partial^2 S(x'', t''; x', t')}{\partial x'' \partial x'}.$$
(20)

One can check that $\omega(t)$ actually obeys (19) with initial condition $\omega(t') = 1$, thanks to (8) and (14). So equation (20) implies that (17) indeed coincides with (4).

Although all (continuous) paths joining (x', t') with (x'', t'') seem to enter the Feynman path integral (1), only a certain subset of fractal paths with Hausdorff dimension 2 (namely for which $\Delta x(t) \sim (\Delta t)^{1/2}$) actually contribute (Feynman and Hibbs 1965)—they are the so-called Feynman paths. A very similar situation occurs for the new path integral (6) and those paths which actually contribute in (6) will be referred to as generalized Feynman paths. No connection is known to exist between the Feynman paths and the classical dynamical trajectories in \mathcal{M} . Yet, the generalized Feynman paths have a very simple relation to the classical dynamical trajectories in \mathcal{M} . Even though this issue will be discussed in great detail elsewhere (Roncadelli 1992a), one can perhaps be convinced of this fact by simply noticing the very strong structural similarity between equation (12) and the exponent in the path integral (6).

A more detailed discussion of the new path integral will be presented in a forthcoming paper (Roncadelli 1992b).

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