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Quantum first-passage problem*

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Abstract. Formulation of quantum first passage problem is attempted in terms of a restricted Feynman path integral that simulates an absorbing barrier as in the corresponding classical case. The positivity of the resulting probability density, however, remains to be demonstrated.

Keywords. First passage; path decomposition; absorbing barrier; traversal time; collapse of wave function; Stochastic quantization.

In a quantum first-passage problem (QUIPP) one is interested in the probability of the occurrence of a certain event of interest in a time interval $[t, t+\Delta t]$ for the *first* time, given that the system was prepared at $t = 0$ in a prescribed initial state φ_i. The first passage problem is a well-known, well-posed and solvable problem in classical probability theory and theory of Markovian stochastic processes (Chandrasekhar 1943; Weiss 1967). Its study is well motivated in that the first passage may be the rate-limiting step in an activated chemical reaction involving escape over barrier followed by efficient removal (scavenging) of the escaping species by a reactant idealized as an absorbing barrier. Thus the mean-first-passage-time should be of considerable significance in calculating the reaction rates (Weiss 1967). However, to the best of the author's knowledge, there is no corresponding treatment of QUIPP in the literature. Indeed, in the course of several informal discussions the author has had in recent years with other workers, it turned out that the QUIPP is generally believed to be an ill-posed problem because of the nature of quantum probability which is linked intimately to the measurement theory. Thus for the case of a two-state system one argues, and rightly so, that QUIPP would necessitate, in principle, a continuous observation on the system. This would imply infinitely often repeated observations resulting in the blocking of evolution of the state of the system by the repeated collapse of the wave function (Simonius 1978). A possible, if indirect, approach to QUIPP seems to be the one based on stochastic quantization (Weaver 1978; Nelson 1966). Since the equivalence of stochastic quantization to standard quantum mechanics is still in question, it is desirable to have a solution of QUIPP directly in terms of standard quantum mechanics. Thus motivated, we present the following formulation and solution of QUIPP in terms of a constrained Feynman path integral that seems most naturally suited to this problem. Such a constrained (restricted) path integral has been introduced recently by Auerbach *et al* (1984) in a different context for their path decomposition expansion scheme.

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To fix ideas and for the sake of clarity, let us begin by considering the simplest classical stochastic process, namely the Wiener process described in one dimension by

$$dX = f(t)\,dt, \tag{1}$$

where $f(t)$ is assumed gaussian and delta-correlated, i.e., $\langle f(t)f(t')\rangle = 2D\delta(t-t')$. It is known that X is then a Markovian process with the probability density $\rho(X,t)$ satisfying the diffusion equation

$$(\partial\rho/\partial t) = D(\partial\rho^2/\partial X^2) \tag{2}$$

and the associated transition probability (Greens function) $K_{cl}(X_2, t_2; X_1, t_1)$ is

$$K_{cl}(X_2, t_2; X_1, t_1) = \frac{1}{[4\pi D(t_2-t_1)]^{1/2}} \exp[-(X_2-X_1)^2/4D(t_2-t_1)] \qquad t_2 \geqslant t_1. \tag{3}$$

This transition probability has the Feynman-Kac path integral representation

$$K_{cl}(X_2, t_2; X_1, t_1) = \int D[X(t)] \exp\left[-\frac{1}{4D}\int_{X_1(t_1)}^{X_2(t_2)} (dX/dt)^2\,dt\right] \tag{4}$$

This is an unrestricted sum over all paths, each path weighted by a certain factor. Now we can introduce the constrained (restricted) path integral as the one obtained by summing over a subset of all possible paths. For the classical first-passage problem, thus, one defines the restricted propagator $K_{cl}^{(r)}(X_2, t_2; X_1, t_1|X)$ by summing over only those paths $X_1, t_1 \to X_2, t_2$ that do not cross the point $X > X_1, X_2$. That is

$$K_{cl}^{(r)}(X_2, t_2; X_1, t_1|X) = \int_{X^{(r)}(\cdot)} D[X(t)] \exp\left[-\frac{1}{4D}\int_{X_1(t_1)}^{X_2(t_2)} dt\left(\frac{dX}{dt}\right)^2\right], \tag{5}$$

where $X^{(r)}(\cdot)$ denotes a path restricted such that $x(t) < x$ for $t_1 \leqslant t \leqslant t_2$. The point to note is that $K_{cl}^{(r)}$ obeys the same diffusion equation as K_{cl}, the latter being a local property. Thus the constraint (restriction) on the set of paths to be counted in evaluating the path integral (5) is equivalent to imposing a certain boundary condition for the associated differential equation (2). The first passage probability $P_{cl}^{(I)}(x, t/X_1, t_1)$ is now given by

$$P_{cl}^{(I)}(X, t|X_1, t_1) = -\frac{\partial}{\partial t}\int_{-\infty}^{X} K_{cl}^{(r)}(X', t; X_1, t_1|X)\,dX' \tag{6}$$

Here $P_{cl}^{(I)}(X, t/X_1, t_1)\Delta t$ gives the probability that the particle starting at X_1, t_1 will cross X in the time interval $[t, t+\Delta t]$ for the *first* time. The key object to calculate is then $K_{cl}^{(r)}(X_2, t_2; X_1, t_1|X)$. For this one has to solve the Greens function associated with the diffusion equation (2) subject to the absorbing boundary condition at X. This is done readily by the method images (Chandrasekhar 1943). In the present case, one could write

$$K_{cl}^{(r)}(X_2, t_2; X_1, t_1|X) = K_{cl}(X_2, t_2; X_1, t_1) - K_{cl}^{(\bar{r})}(X_2, t_2; X_1, t_1|X) \tag{7}$$

where $(\bar{r})$ denotes complementary constraint, i.e., it counts only paths for which the particle crosses the point X at least once. Now one can readily see that

$$K_{cl}^{(\bar{r})}(X_2 t_2; X_1 t_1|X) = K_{cl}(2X - X_2, t_2; X_1 t_1),$$

for there is one-to-one correspondence between paths counted in these two path integrals. This together with (3), (6) and (7) gives the well-known expression for the first-passage probability (Weiss 1967). It also gives the boundary condition

$$K_{\mathrm{Cl}}^{(r)}(X_2, t_2; X_1 t_1 | X) \to 0 \text{ as } X_2 \to X. \tag{8}$$

We are now ready to adapt this classical calculation to the case of QUIPP. But first we must note the all important difference between the classical transition probability (3) and the quantum transition amplitude given by the Feynman path integral K_Q as

$$K_Q(X_2, t_2; X_1, t_1) = \int_{t_2 \geqslant t_1} D[X(t)] \exp\left[\frac{i}{\hbar}\int_{X_1(t_1)}^{X_2(t_2)} L(X, \dot{X})\,\mathrm{d}t,\right. \tag{9}$$

with $L = \frac{1}{2}m\dot{X}^2 - V(X)$. The path-integral decomposition (4) of the classical transition probability is *real* in the sense that each path is a possible realization of the stochastic process with prescribed additive probability and one could actually track these Brownian paths traversed by the particle. In contradistinction with this the path-integral decomposition of the quantum transition amplitude (9) is purely a mathematical construction (virtual) in that such a space-time trajectory is not admitted in quantum mechanics. We believe, however, that the following remains true even in the quantum case: Namely, that the *restricted* (r) Feynman path integral $K_Q^{(r)}$ will lead to a correspondingly *restricted* transition probability. (This is because the inclusion of the complementary ($\bar{r}$) paths should at the very least make the calculated probability depend on any test (scalar) potential $V(X')$ that may be there for $X' > X$. To sense this potential the particle must have really been there. This test of *reality* is akin to that used for traversal time in quantum mechanics where an internal spin-moment senses the test magnetic field and thus clocks the time). Here again the restriction (r) denotes that only paths that stay to the left of X are to be summed over. Thus, if the particle was prepared initially in state φ_i, the evolved wave function $\varphi^{(r)}$ subject to the restriction (r) will be

$$\varphi^{(r)}(X_2, t_2) = \int_{-\infty}^{X} \varphi_i(X') K_Q^{(r)}(X_2, t_2; X', t_1 | X)\,\mathrm{d}X_1 \tag{10}$$

Here one assumes naturally that $\varphi_i(X')$ is non-zero only for $X' < X$. Then the QUIPP is solved by

$$P_Q^{(l)}(X, t | \varphi_i) = -\frac{\partial}{\partial t}\int_{-\infty}^{X} |\varphi^{(r)}(X', t)|^2\,\mathrm{d}X' \tag{11}$$

As before, $K_Q^{(r)}$ and hence $\varphi^{(r)}$ obey the original Schrödinger equation. The only remaining question is how to evaluate the restricted propagator $K_Q^{(r)}(X_2, t_2; X_1, t_1 | X)$. In terms of the boundary condition the question is how to impose the equivalent of absorbing boundary condition at X. Since the quantum-mechanical probability current is bilinear in the wave function and its gradient, we may not impose, as in the classical case, that $K_Q^{(r)}(X_2, t_2, X_1 t_1 | X)$ should vanish as $X_2 \to X$. This would lead to total confinement as if we had an infinite potential barrier. The allowed boundary condition can be found by the following procedure where $K_Q^{(r)}(X_2, t_2; X_1, t_1 | X)$ is imbedded in $K_Q(X_2, t_2; X_1, t_1)$ with $X_2 > X \geqslant X_1$ leading to an integral equation for $K_Q^{(r)}$. To this end one counts the paths contributing to $K_Q(X_2, t_2; X_1, t_1)$ *and re-order the paths* $X(.)$ *according to increasing time of first-passage through* X. Thus the paths that cross X in

the time-interval $t-\varepsilon/2$ to $t+\varepsilon/2$ for the first time contribute

$$K_Q\left(X_2, t_2; X, t-\frac{\varepsilon}{2}\right)K_Q^{(r)}\left(X, t-\frac{\varepsilon}{2}; X_1, t_1 \mid X\right)$$

$$-K_Q\left(X_2, t_2; X, t+\frac{\varepsilon}{2}\right)K_Q^{(r)}\left(X, t+\frac{\varepsilon}{2}; X_1, t_1 \mid X\right)$$

$$X_2 > X; X_1 \leqslant X. \tag{12}$$

Summing over all such time-intervals, letting $\varepsilon \to 0$ and taking the Fourier transform with respect to $t_2 - t_1$, we get

$$\tilde{K}_Q(X_2, X_1; E) = \tilde{K}_Q(X_2, X; E)\left(\frac{i\hbar}{2m}\right)\frac{\partial}{\partial X}\tilde{K}_Q^{(r)}(X, X_1; E|X)$$

$$-\tilde{K}_Q^{(r)}(X, X_1; E|X)\left(\frac{i\hbar}{2m}\right)\frac{\partial}{\partial X}\tilde{K}_Q(X_2, X; E) \tag{13}$$

in obvious notation. This gives the condition that the right side must vanish for $X_2 \to X_1' < X$, i.e.

$$\tilde{K}(X_1', X; E)\frac{\partial}{\partial X}\tilde{K}_Q^{(r)}(X, X_1; E/X)$$

$$-\tilde{K}_Q^{(r)}(X, X_1; E|X)\frac{\partial}{\partial X}\tilde{K}_Q(X_1', X; E) = 0 \tag{14}$$

Equation (14) provides the boundary condition for the restricted propagator $K_Q^{(r)}(X_2, X_1; E|X)$ defined for $X_2 < X; X_1 \leqslant X$. Letting X_2 approach arbitrarily close to X and recalling that the unrestricted propagator for small spatial separation becomes essentially the free propagator, we get (Auerbach *et al* 1984)

$$-i\hbar\frac{\partial}{\partial X_1'}\ln\tilde{K}_Q^{(r)}(X_1', X_1; E/X) = [2m(E-V(X)]^{1/2} \lim X_1' \to X. \tag{15}$$

One can easily interpret (15) as the quantum analogue of the absorbing boundary condition as it admits only the right-moving wave at the boundary X. This completes the derivation.

Several comments are now in order. First, we note that the boundary condition (15) is *not self-adjoint*. This seems to corroborate with the impossibility of finding a self-adjoint operator corresponding to the first-passage time regarded as an observable Allcock (1969). Secondly, as mentioned before, for the discrete case of two-state problem, say, the first passage time will operationally require a state-sensitive ideal detector which is 'on' all the time, i.e. continuous measurement of the first kind in the von Neumann sense, leading to blocking of evolution, and hence no first-passage. I think this is so, because, for the discrete (essentially finite dimensional) case, there is no distinction between the hermitian and the self-adjoint operators unlike the continuum case considered here. Also, the real space-time path integral treatment does not exist for such discrete cases. Perhaps one would need a non-demolition type of detection. Finally, there is the question of the positivity of the first-passage probability given by (11). Incorporating the boundary condition (15) in the time domain via the identity

$$\frac{d^{1/2}}{dt^{1/2}}f(t) = \frac{1}{\sqrt{\pi}}\frac{d}{dt}\int_0^t \frac{f(\tau)}{\sqrt{t-\tau}}d\tau,$$

we can re-write (11) as

$$P_Q^{(I)}(X,t\,|\,\varphi_i)=\left(\frac{\hbar}{4\pi m}\right)^{1/2}(1+i)Q^{*(r)}_{(X,t)}\int_0^t\frac{\mathrm{d}\varphi^{(r)}_{(X,\tau)}}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\sqrt{t-\tau}}+\text{c.c.} \tag{16}$$

We have not been able to establish the positivity of this quantity. However, for the simple case of a free particle confined to half-line ($0 \leqslant X < \infty$) and prepared initially in a spatially narrow wave-packet φ_i of width ε centred at $X_0 < X$, we get

$$P_Q^{(I)}(X,t/\varphi_i)\simeq\sqrt{\frac{2}{\pi}}\left(\frac{m\varepsilon}{\hbar}\right)\left(\frac{x}{t^2}\right)\cdot\left(1+\cos\left(\frac{2m}{\hbar}\frac{x_0x}{t}\right)\right), \tag{17}$$

for $\qquad \varepsilon \ll X_0, t \gg 2m\varepsilon^2/\hbar.$

This certainly stays positive. But in general we do not know yet. Further work is in progress.

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