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A STOCHASTIC DESCRIPTION OF TUNNELING IN QUANTUM MECHANICS

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Quantum theory and classical probability theory have some structures in common from which the development of quantum theory has sometimes benefited. The best known connection between them is that Euclidean (i.e. imaginary time) quantum theory coincides with the theory of diffusion in real time. Hence by means of the Euclidicity postulate one can transform the characteristic differential equations of probability theory as well as the descriptions in terms of functional intengrals into quantum theory.(1)

The purpose of this lecture is to discuss an interesting area of overlap, namely tunneling phenomena, where the theory of stochastic processes offers some relief in the difficult problem of computing functional determinants.(2) In the standard method of recovering transition probabilities from the functional integral

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one comes inevitably against this difficulty. There is in principle a different approach towards the recovery of transition probabilities from the generating functional which avoids Gaussian integrals. It consists in first defining out of the generating functional other functionals (sections) which, besides normalisation, are semi-continuous and positive-definite. These properties are sufficient to activate Böchner's theorem which then allows to obtain the transition probabilities as Fourier transforms of the sections. I will not follow this approach here. Our main observation is that tunneling phenomena in quantum theory, whether ot not one looks at them as transitions associated with instantons and anti-instantons[3] may be modeled by a birth and death counting (Poisson) process. The problem of computing the functional determinant is reduced, via this modeling, to the much simpler problem of finding the average waiting time of the counting process.[2] There is a simple formula connecting the two.

Let us start by considering the description of tunneling in quantum mechanics. From the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} + V(x)\varphi(x) = E\varphi(x) \qquad (1)$$

one obtains, by introducing the drift velocity

$$T(x) = \frac{\hbar}{m}\frac{d}{dx}\ln\varphi(x) \qquad (2)$$

the Riccati equation

$$\frac{\hbar}{2}\frac{dT(x)}{dx} + \frac{m}{2}T^2(x) = V(x) - E \qquad (3)$$

The solution of the original Schrödinger equation is now sought by solving (3) by iteration:

$$T_o(x) = \pm \left[\frac{2}{m} (V(x) - E) \right]^{1/2} \tag{4}$$

$$= \pm \frac{i\hbar}{m} k(x) = \pm \frac{\hbar}{m} K(x)$$

K(x) is real where V(x) > E and purely imaginary in those regions where V(x) < E. The n-th iterate is

$$T_n(x) = \left(T_o^2(x) - \frac{\hbar}{m} \frac{dT_{n-1}(x)}{dx}\right)^{1/2}$$

$$\simeq T_o(x) - \frac{\hbar}{2m} \frac{1}{T_o(x)} \frac{dT_{n-1}(x)}{dx} \tag{5}$$

The first iterate (the negative sign in eq (4) gives a normalisable wave function)

$$T_1(x) \simeq - \frac{\hbar}{m} K(x) - \frac{\hbar}{2m} \frac{d}{dx} m K(x) \tag{6}$$

gives the WKB approximation. Let $\psi(x)$, through eq (2), be the corresponding wave function. One finds the well known result.

$$\psi(x) = \frac{1}{\sqrt{K(x)}} \exp\left(- \int^{x} dy K(y) \right) \tag{7}$$

Contrary to quantum mechanics the theory of stochastic processes invests considerably more attention in the study of the consequences of the zeroth solution $T_o(x)$. It gives the so-called deterministic solution for the velocity, which in the Euclidean space description (τ = it) is given by

$$\frac{dx(\tau)}{d\tau} = T_o(x) \tag{8}$$

$x(\tau)$ will always stand for the classical (i.e. deterministic) path. The reason for the special interest of stochastic mechanics in eq.(8) is that some of the equilibria of the physical system which is being described are the singular points of eq.(8). These are the zeros of $T_o(x)$; i.e. the points $x_n (n=1,2,...)$ with

$$T_o(x_n) = 0; \quad n = 1, 2, ... \tag{9}$$

Systems for which eq.(9) defines equilibrium are usually dissipative, dissipation occuring through the drift. The equilibria are absorptive, that is once the system relaxes into any one of these states it remains there indefinitely. Random fluctuations alone cannot drive the system into another equilibrium state. The problem of tunneling does not exist for such systems.

For conservative systems on the other hand, force does more than just impart a velocity; it produces acceleration so that equilibrium is not defined by eq.(9). For these systems equilibria are all orbits of uniform velocity (including zero velocity) i.e. the points x_n (n = 1,2, ...) where

$$\left(\frac{dT_o(x)}{dx}\right)_{x=x_n} = 0, \quad n = 1, 2, ... \tag{1o}$$

The absorptive equilibria (those x_n with $T_o(x_n) = 0$ in addition to (1o)) constitute therefore only a subset of all the equilibrium states. Nonabsorptive equilibria are called transients. Random fluctuations

alone can induce transitions between them, even when in Minkowski space - time these transitions are not deterministically possible.
Equilibrium sates which are so related are said to be communicating. Communication is an equivalence relation in the set of transient equilibria. An equivalence class is called a chain. The problem of tunneling in quantum mechanics has thus been transformed into one in stochastic mechanics.

Consider then the chain spanned by a countable number of states labelled by integers (both positive and negative for instance). Transitions in the chain consist then in a time-dependent step-up (birth) and step-down (death) of the integer coordinates. We shall assume that these are Poisson processes. What is the relationship between this description and the solutions of the Riccati equation through which one recovers the description in terms of wave functions? In other words, how does one measure the effect of the random fluctuations responsible for transitions in the chain?

Let $q(\tau)$ be the stochastic process with drift velocity $T(q)$ and diffusion coefficient $\nu = \hbar/2m$ for which the Riccati equation (eq.(3) constitutes the first integral of the action of the corresponding generator

$$\left(T(x) \frac{d}{dx} + \frac{\hbar}{2m} \frac{d^2}{dx^2}\right) T(x) = \frac{1}{m} \frac{dV(x)}{dx} \tag{11}$$

$q(\tau)$ satisfies the Langevin equation

$$dq(\tau) = T(q)\, d\tau + dw(\tau) \tag{12}$$

where $dw(\tau)$ is a Wiener process.

$$\begin{aligned} \langle dw(\tau)\rangle &= 0 \\ \langle dw(\tau_2)\ dw(\tau_1)\rangle &= \frac{\hbar}{m}\,|\tau_2 - \tau_1| \end{aligned} \qquad (13)$$

Any transient equilibrium perturbed by $dw(\tau)$ is rendered unstable after some (random) time. For vanishing diffusion coefficient, that is, for $\hbar \to 0$, the probability for the system to pass from a state $q(\tau_1) = x_1$ to $q(\tau_2) = x_2$ in the time $\tau = \tau_2 - \tau_1$ is measured by the function

$$\begin{aligned} w(\tau_2, x_2|\tau_1 x_1) &= \exp(-E(\tau_2-\tau_1)/\hbar)\cdot \\ &\cdot \exp\left[-\frac{m}{2\hbar}\int_{\tau_1}^{\tau_2} d\tau\left(\frac{d\dot{q}(\tau)}{d\tau} - T_0(q(\tau)\ )\right]\right. \end{aligned} \qquad (14)$$

Using eqs (2) and (3) in (14), $w(\tau_2, x_2|\tau_1 x_1)$ becomes

$$w(\tau_2, x_2|\tau_1, x_1) = \frac{\varphi_0(x_2)}{\varphi_0(x_1)} \exp\left(-\frac{1}{\hbar} S_E(\tau_1, \tau_2)\right) \qquad (15)$$

where $\varphi_0(x)$ is obtained from eq (2) with $T(x) \equiv T_0(x)$ and

$$\begin{aligned} S_E(\tau_2, \tau_1) &= \int_{\tau_1}^{\tau_2} d\tau\left(\frac{m}{2}\left(\frac{dq}{d\tau}\right)^2 + V(q)\right) \qquad (16) \\ &\equiv \int_{\tau_1}^{\tau_2} d\tau\ H\ (q(\tau),\ \dot{q}(\tau)) \end{aligned}$$

is the Euclidean action of the classical problem associated with the Schrödinger Hamiltonian in eq(1). $H\ (q(\tau),\ \dot{q}(\tau))$ is the corresponding Hamiltonian.

Now the characteristics of the distribution of random times at which transitions occur are those of the Poisson processes in the Markov chain. So let $P_{n,n+1}(\tau)$ be the probability of a birth (B) in time τ $P_{n,n-1}(\tau)$ the probability for death (D) and $P_{n,n}(\tau)$ the probability for permanence in the same state n after time τ . From the assumption that transition processes are Poissonian we have in a short time interval $\Delta\tau$

$$
\begin{aligned}
P_{n,n+1}(\Delta\tau) &= \lambda\Delta\tau + O[(\Delta\tau)^2] \\
P_{n,n-1}(\Delta\tau) &= \lambda\Delta\tau + O[(\Delta\tau)^2] \\
P_{n,n}(\Delta\tau) &= 1 - 2\lambda\Delta\tau + O[(\Delta\tau)^2]
\end{aligned}
\qquad (17)
$$

For simplicity we have assumed the same rate λ for both birth and death. Birth and death processes are in competition in activating the chain. The probability for a transition in time τ from a given initial state n to a final state n + N is therefore given by the conditional probability

$$
\begin{aligned}
T_{n,n+N}(\tau) &= \frac{\Pr(B(\tau)=n_+, D(\tau)=n_- \mid B(\tau)-D(\tau)=N)}{P_{n,n}(\tau)} \\
&\equiv \sum_{n_-,n_+=0}^{\infty} \delta((n_+-n_-)-N) \cdot \frac{P_{n,n+n_+}(\tau)\, P_{n,n-n_-}(\tau)}{P_{n,n}(\tau)}
\end{aligned}
\qquad (18)
$$

From the integration of eq(17) we have the finite probabilities

$$P_{n,n+n_+}(\tau) = \frac{(\lambda\tau)^{n_+}}{(n_+)!} \quad e^{-\lambda\tau}$$

$$P_{n,n-n_-}(\tau) = \frac{(\lambda\tau)^{n_-}}{(n_-)!} \quad e^{-\lambda\tau} \qquad (19)$$

$$P_{n,n}(\tau) = e^{-2\lambda\tau}$$

Substituting (19) into (18) gives [3]

$$T_{n,n+N}(\tau) = \frac{1}{2\pi}\int_0^{2\pi} d\theta e^{-iN\theta} \exp(\lambda\tau\cos\theta)$$

$$\equiv \frac{1}{2\pi}\int_0^{2\pi} d\theta \langle n+N|\theta\rangle\langle\theta|e^{-H\tau/\hbar}|n\rangle \qquad (2o)$$

where the Hamiltonian H is the integrand of eq (16). Transitions from the discrete states $|n\rangle$ of the chain into the continuous set of intermediate states $|\theta\rangle$ are given by the matrix elements

$$\langle n+N|\ \theta\rangle = e^{-i(n+N)\theta}$$

$$\langle\theta|e^{-H\tau/\hbar}|n\rangle = e^{-E(\theta)\tau/\hbar} \ e^{in\theta} \qquad (21)$$

$$E(\theta) = -\hbar\lambda\cos\theta$$

Eq (2o) contains the unknown parameter λ. Its physical meaning is, however, clear from both the point of view of the counting processes and that of the difference in energies between the perturbed states. We will now show how it may be related to a time average over the distribution $w(\tau_2,x_2|\tau_1,x_1)$. To this end let σ be the first arrival time of the Poisson processes, i.e. the first time a birth or a death occurs. σ is exponentially distributed:

$$f\ (\sigma) \quad = \quad \lambda e^{-\lambda\sigma} \tag{22}$$

The probability for just <u>one</u> transition to occur is therefore proportional to the integral

$$I = \int_0^\infty d\sigma f(\sigma) \int_{\tau_1}^{\tau_1+\sigma} d\tau_2 \frac{dq(\tau_2)}{d\tau_2} \quad w(\tau_2, q(\tau_2) \,|\, \tau_1, x_1) \tag{23}$$

$$= \int_0^\infty d\sigma f(\sigma) \int_0^\sigma d\tau \frac{dq(\tau)}{d\tau} \quad w(\tau, q(\tau) \,|\, 0, x_1)$$

The constant of proportionality, N, is given by the normalisation

$$N \int_0^\infty d\tau \frac{dq(\tau)}{d\tau} \, w(\tau,\, q(\tau) \,|\, 0,\, x_1) = 1 \tag{24}$$

of the total transition probability out of the state x_1. The average waiting time at the state x_1 (i.e. its mean life time) is therefore given by

$$\frac{1}{\lambda} = \frac{\displaystyle\int_0^\infty d\sigma f(\sigma) \int_0^\sigma d\tau \; \tau \frac{dq(\tau)}{d\tau} \quad w(\tau, q(\tau) \,|\, 0,\, x_1)}{\displaystyle\int_0^\infty d\tau \frac{dq(\tau)}{d\tau} \, w(\tau, q(\tau) \,|\, 0, x_1)} \tag{25}$$

The evaluation of the integrals in eq (25) is well known; one uses eqs (15) and (16) for $w(\tau,q(\tau)|\,O,x_1)$ and expands $S_E(\tau,O)$ about a classical path. The classical path in the time interval (O,σ) is just x_1. The mean value theorem is used to simplify the calculation. A Gaussian integral results from the use of eq (13) to replace $[\delta q(\tau)]^2$ by

$$<[\delta q(\tau)]^2> \quad = \quad \frac{h}{m}\tau + O(\tau^2) \tag{26}$$

for small τ. The final result is

$$\left(\frac{\delta^2 H}{\delta x^2}\right)^{-1/2} = \left[\det\left(-\frac{md^2}{d\tau^2} + \frac{d^2V(x)}{dx^2}\right)\right]$$

$$= \frac{1}{\lambda}\left(\frac{\pi}{m}\right)^{1/2} e^{-S_E/h} \tag{27}$$

The functional determinant has thus been evaluated without encountering the problem of zero eigenvalues. The exact value of the rate λ is not required. It can be absorbed into a normalisation constant[3]. The reader can easily verify that eq (27) gives the familiar result for the harmonic oscillator. The classical action in this case is found by applying the ergodic theorem

$$S_E(T,O) = \int_O^T d\tau\left[\frac{m}{2}\left(\frac{dq}{d\tau}\right)^2 + \frac{m}{2}\omega^2 q^2\right]$$

$$= m\omega^2 T \lim_{T\to\infty}\frac{1}{T}\int_O^T d\tau q^2(\tau)$$

$$= m\omega^2 T \quad < q^2 >$$

$$= \frac{\hbar\omega}{2} T \tag{28}$$

Although, we have considered here only the one dimensional Schrödinger equation the extension to more dimensions and to field theory is fairly straight - forward.

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