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352

Path Integral Approach to Interaction and Tunneling Times

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Abstract

The path integral approach is used to formulate the interaction time for a classical as well as for a quantum mechanical, structureless object which interacts with a time-dependent force acting in some prescribed region in space. In doing so, we establish an adiabaticity criterion, both for classical stochastic motion and quantum motion. The quantum case involves two complex-valued time parameters with analogues for the classical Brownian motion. Both parameters reduce semiclassically in magnitude to the well known expression, representing the time of motion along the stationary classical path. By use of a series of distinct observations and other arguments we show that the quest of finding a unique tunneling time seems to be without hope.

1. Introduction

In physical sciences the role of time-scales, particularly the concept of a clearcut separation of various time scales plays an ubiquitous role in describing physical processes. In the following we shall address the role of quantum mechanics and interaction times from a path integral point of view. This work is based on a previous collaboration¹ with Dr. Sokolovski, and closely related work by the latter^{2,3}. In the first part we shall focus on complex-valued interaction times, whereas in a second part the concept of a "tunneling time" will be critically discussed.

In section 2 we first start with the description of the time spent by a classical particle traversing a prescribed interaction region. We note that for an extended classical object there already exists no unique time scale for the "traversal time". By use of two distinct time-averaging procedures we obtain a useful theorem, Eq. (8d). For a classical diffusion process in presence of a coordinate-dependent sink we apply the theorem to obtain a classical adiabaticity theorem for diffusive motion. To deal with the quantum case we rotate time to imaginary values, whereby the diffusion equation goes over into the Schrödinger equation. The classical adiabaticity theorem is then readily generalized to the quantum case. The application of the above theorem then reveals that the result for the interaction time scale can be cast into a product of two different quantum mechanical time scales. It is then natural to ask, what is the correct time for traversal of a quantum mechanical interaction region? This, therefore renders the problem of a quantum tunneling time which we address in section 3. We demonstrate by use of a series of distinct arguments that the quest of finding a unique prescription for the object "quantum tunneling time" is without hope.

2. Interaction Times

Here we consider the time-scale a particle spends in some region of interest, wherein it can interact with a potential, other degrees of freedom, and alike. For the sake of clarity only we assume a one-dimensional configuration space Σ and a time axis \mathcal{T} , describing the dynamics of a particle. A point X=(x,t) out of the direct product space Σ x \mathcal{T} then locates in a unique way a structureless classical particle. Given some interaction region Γ within Σ x \mathcal{T} , see Fig. 1, the characteristic functional θ_{Γ} of a certain prescribed path $\hat{x}(t)$, i.e.

$$\theta_{\Gamma} [\hat{\mathbf{x}}(t)] = \begin{cases} 1 & , \stackrel{\wedge}{\mathbf{X}} = (\stackrel{\wedge}{\mathbf{x}}, t) \in \Gamma \\ 0 & , \stackrel{\wedge}{\mathbf{X}} = (\stackrel{\wedge}{\mathbf{x}}, t) \notin \Gamma \end{cases}$$
 (1)

then defines an interaction time t_T for a structureless point particle moving along $\hat{x}(t)$ given by

$$t_{\Gamma} \begin{bmatrix} \hat{x} \end{bmatrix} = \int_{t_0}^{t_f} \theta_{\Gamma} \begin{bmatrix} \hat{x} \\ t \end{bmatrix} dt = \int_{t_0}^{t_f} dt \int_{x_{<}}^{x_{>}} dx \delta \left[x - \hat{x}(t) \right] . \tag{2}$$

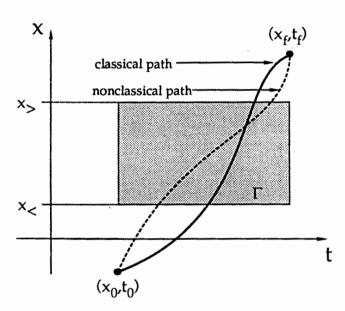


Figure 1: Various paths and the region Γ which are part of the definition of the (path-dependent) time spent in the interaction region, see Eq. (2).

Here t_o denotes the starting point (in time) for $\hat{x}(t)$ and t_f the final time, respectively. Given a point particle, moving along its classical trajectory $x_{cl}(t)$, the above expression yields the classical time t_r^{cl} spent in the interaction region Γ . Already at this classical level we encounter a first difficulty in defining uniquely the interaction time. Suppose we deal with an extended classical object; then the time scale defined as the interaction time which the center-of-mass (c.m.) spends within the region Γ does not equal the time difference for the rear of the object to leave the region Γ at a later time and for the front to enter Γ (see Fig. 2). Given the quantum mechanical uncertainty to measure the coordinate for a point particle it should not come as a surprise for the reader (see below) that no exact, and nonfluctuating value exists for the interaction time of a structureless quantum mechanical object.

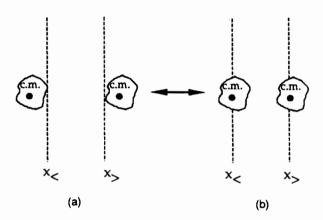


Figure 2: Different possibilities of defining the traversal time for an extended classical object:

(a)
$$t_{\text{tray}}^{(1)} = t_{>}^{\text{rear}} - t_{<}^{\text{front}}$$
; (b) $t_{\text{tray}}^{(2)} = t_{>}^{\text{c.m.}} - t_{<}^{\text{c.m.}}$.

A. A useful theorem

Following Reference 1 we shall next consider random classical trajectories of a diffusion process governed by the Fokker-Planck equation for the probability P_t , i.e.

$$\dot{P}_{t} = \frac{1}{2} \frac{\partial^{2} P_{t}}{\partial x^{2}} - U(x, t) \theta_{\Gamma}(x) P_{t} , \qquad (3)$$

where the initial probability P_{t_0} obeys $P_{t_0}(x) = \delta(x - x_0)$. The propagator $R(x_2 t_2 | x_1 t_1)$, which equals the conditional probability, obeys with $t_f \ge t_n \ge \dots \ge t_1 \ge t_0$ the relation

$$R(x_{f} t_{f} \mid x_{o} t_{o}) = \int \prod_{i=1}^{n} dx_{i} R(x_{f} t_{f} \mid x_{n} t_{n}) R(x_{n} t_{n} \mid x_{n-1} t_{n-1}) \dots$$

$$\dots R(x_{1} t_{1} \mid x_{o} t_{o}) . \tag{4}$$

Within an infinitesimal checker-board discretization the above result can be recast as a path integral,

$$R(x_f t_f | x_o t_o) = \int_{x_o, t_o}^{x_f t_f} \mathcal{D} x(\bullet) \exp(-S [x(\bullet)]) , \qquad (5a)$$

where

$$S[...] = \int_{t_0}^{t_f} \left\{ \frac{\dot{x}^2}{2} + U(x, t) \theta_{\Gamma}[x(t)] \right\} dt .$$
 (5b)

The interaction time t_{Γ} presents a functional of the corresponding trajectory $\hat{x}(t)$. In terms of the two conditional averages defined in (I) and (II), namely given a functional $F[x(\bullet)]$ we define the first average as

(I)
$$\langle F[x(\bullet)] \rangle = \int_{x_0, t_0}^{x_f, t_f} \mathcal{D} x(\bullet) F[x(\bullet)] \exp(-S[x(\bullet)]) / R(x_f t_f \mid x_0 t_0)$$
, (6)

and given a function f(x, t) we define the second average

(II)
$$\overline{f(x, t)} \equiv \int_{\Gamma} f(x, t) d\mu / \int_{\Gamma} d\mu$$
 , (7a)

where dµ denotes the measure

$$d\mu = R(x_f t_f; xt \mid x_o t_o) dx dt$$

$$= R(x_f t_f \mid xt) R(xt \mid x_o t_o) dx dt . \tag{7b}$$

Given (I) and (II) we readily can prove the following theorem

$$< \int_{t_0}^{t_f} f[x(t), t] \theta_{\Gamma}[x(t)] dt >$$

$$= R^{-1} \left(x_f t_f \mid x_o t_o \right) \int \mathcal{D} x(\bullet) \int_{t_o}^{t_f} dt f[x(\bullet), \bullet] \int_{x_{<}}^{x_{>}} \delta[\lambda - x(\bullet)] d\lambda \exp(-S[x(\bullet)]) . (8a)$$

With $Z \equiv \int_{\Gamma} R(x_f t_f | \lambda t) R(\lambda t | x_o t_o) d\lambda dt$, one can write further

$$= R^{-1}(x_f t_f \mid x_o t_o) Z \left\{ Z^{-1} \int_{\Gamma} d\lambda dt f(\lambda, t) R(\lambda t \mid x_o t_o) R(x_f t_f \mid \lambda t) \right\} . \quad (8b)$$

Unfolding the term "Z" into a single path-integral again we find upon noting that the term in the curly brackets yields the conditional average (II)

$$= \overline{f[x(t), t]} \left[R^{-1} \left(x_f t_f \mid x_o t_o \right) \int_{x_o, t_o}^{x_f, t_f} \mathcal{D} x(\bullet) \int_{t_o}^{t_f} dt \int_{x_c}^{t_f} d\lambda \, \delta[\lambda - x(\bullet)] \exp(-S[x(\bullet)]) \right] (8c)$$

which equals our main result

$$< \int_{t_0}^{t_f} f[x(t), t] \theta_{\Gamma}[x(t)] dt > = \overline{f[x(t), t]} < t_{\Gamma}[x(\bullet)] > .$$
 (8d)

In other words, the conditional average in Eq. (8a) separates into two conditional averages where the 2-nd part in Eq. (8d) denotes the average of the interaction time of a random trajectory $x_{\omega}(t) \equiv x(\bullet)$ of the diffusive process in Eq. (3); see Fig. 1.

B. Adiabaticity criterion for classical diffusion

As a first application of the theorem in Eq. (8d) we look for a criterion under which we can substitute the time-dependent interaction U(x,t) by a time-independent function $\hat{U}(x) \equiv U(x, t = \hat{t})$ where we "freeze" the interaction at some time point \hat{t} . If we treat the difference $[U(x, t) - \hat{U}(x)]$ as a perturbation we find in leading order

$$R(x_{f} t_{f} \mid x_{o} t_{o})_{U(x, t)} \sim R(x_{f} t_{f} \mid x_{o} t_{o})_{\hat{U}}$$

$$\left[1 - \left\langle \int_{t_{0}}^{t_{f}} \theta_{r} \left[x(t)\right] \left[U(x, t) - \hat{U}(x)\right] dt \right\rangle_{\hat{U}} \right] . \tag{9}$$

Thus, in virtue of Eq. (8d) we find for the validity of the adiabatic approximation the criterion

$$\gamma = \left| \left\langle \int_{t_0}^{t_f} \theta_{\Gamma} \left[U - \hat{U} \right] dt \right\rangle_{\hat{U}} \right|$$

$$= \left| \overline{\left[U(x, t) - \hat{U}(x) \right]} \right\langle t_{\Gamma} \left[x(\bullet) \right] \right\rangle_{\hat{U}} \left| \left\langle \left\langle 1 \right\rangle \right\rangle. \tag{10}$$

The quantity " γ " thus presents a measure for the validity of the adiabatic approximation, which in turn involves the average over the random trajectories of the classical time spent inside the interaction region. Note that the average $\langle t_{\Gamma}[x(\bullet)] \rangle$ is real valued in this case. For the special case of an oscillating interaction $U(x, t) = \theta_{\Gamma} U_{o} \cos \omega_{o} t$ we obtain with $\hat{t} \equiv t_{f}$, upon an expansion to first order in U_{o} , and $(t - t_{f})$ the result

$$\gamma = \omega_{o} U_{o} \left| \frac{1}{(t - t_{f})} < t_{\Gamma} [x(\bullet)] > 1 \right|$$

$$\equiv \omega_{o} \left| t_{ad}^{\text{diffusion}} \right| << 1 .$$
(11)

C. Adiabaticity criterion for the quantum dynamics

By use of a Wick-rotation in time, i.e. $t \rightarrow + i t$, the diffusion equation is closely related to the Schrödinger equation

In contrast to the stochastic classical situation, we now have to deal with complex quantities. The exponent in the corresponding path integration formula for the propagator thus becomes a complex-valued expression, $S \rightarrow S = -(i/\hbar) \int_{t_0}^{t_f} \left\{ m \frac{\dot{x}^2}{2} - U(x, t) \theta_{\Gamma}(x) \right\} dt = -(i/\hbar) S$. The corresponding quantum adiabaticity criterion $\gamma_{q, m}$ can be readily obtained from the previous results in Eq. (10) and Eq. (11). For the oscillating potential we thus obtain

$$\gamma_{q,m.} = \omega_o \cdot \frac{U_o}{\hbar} \left| (\overline{t_f - t}) < t_{\Gamma} [x(\bullet)] > \right|$$
 (13a)

$$= \omega_{o} \left| < \frac{U_{o}}{\hbar} \int_{t_{o}}^{t_{f}} (t_{f} - t) \theta [x(t)] dt > \right|$$
 (13b)

$$\equiv \omega_{o} \mid t_{ad}^{q.m.} \mid << 1 . \tag{13c}$$

This quantum mechanical "adiabatic time scale" $t_{ad}^{q,m}$ is therefore complexvalued. The criterion involves its absolute value. From Eq. (13a) we note that $t_{ad}^{q,m.}$ involves two complex-valued time scales. The first one, $(\overline{t_f - t})$, involves the complex-valued average of Eq. (7a) for the time argument of the propagator, i.e. t; whereas the second time scale just coincides with the complex-valued traversal time introduced by Sokolovski and Baskin², i.e.

$$t_{\Gamma}^{q,m.} \equiv \langle t_{\Gamma} [x(\bullet)] \rangle . \tag{14}$$

In the context of tunneling through an oscillating barrier these two time scales simplify considerably in the limit of an opaque barrier¹. If the energy of the incident particle is fixed at a value $E = (\bar{h} k)^2/2m$, we find in terms of the momentum inside the classically forbidden region

$$\hbar \kappa(x) \equiv \left\{ 2m \left[U(x) - E \right] \right\}^{1/2} ,$$

for the above two time-scales the semiclassical results¹

$$\left| \overline{t(E) - t_f} \right| \sim \frac{1}{2} \int_{x}^{x_{>}} \frac{m dx}{\hbar \kappa(x)} + O(\hbar) ,$$
 (15)

and

$$\left| \begin{array}{ccc} \overline{t(E) - t_f} \right| & \sim & \frac{1}{2} \int\limits_{x_{<}}^{x_{>}} \frac{m dx}{\hbar \kappa(x)} & + O(\hbar) & , \end{array} \right. \tag{15}$$

$$\left| \begin{array}{ccc} t_f^{q.m} \\ \end{array} \right| & \sim & \int\limits_{x_{<}}^{x_{>}} \frac{m dx}{\hbar \kappa(x)} & + O(\hbar) & . \tag{16}$$

Hereby, $\{x_{<}, x_{>}\}\$ denote the classical turning points inside the barrier where E < U(x).

Interestingly enough, the values in Eqs. (15, 16) are both related to the well-known semiclassical (imaginary-valued) time for tunneling through a barrier.

3. Quantum Tunneling Time

The question which loosely formulated reads "how much time does tunneling take" is intriguing and has quite a long history⁴⁻⁸. The question has also been part of textbook discussions (see page 95 in Reference 8.) and recently did undergo a renaissance in the eighties after the popularization of the issue as presented by works of Büttiker and Landauer⁹⁻¹². All this has triggered more intensive and systematic studies and discussions which cumulated in an authoritative critical survey in the "Reviews of Modern Physics" by Hauge and Stovneng¹³. In the following, I shall present some more detailed observations, together with a series of personal viewpoints on the subject of a (unique) traversal- or tunneling-time.

As we have demonstrated, complex-valued quantities with the dimension of time (or frequency) do represent useful theoretical objects. For example, the adiabatic criterion in the previous section 2.C involves the complex-valued object t_{ad}, which in turn is made up of even two further complex valued timescales. Clearly, physical answers, such as the formulation of the criterion $\gamma_{q,m,.}$ involves real-valued objects only; i.e. one has to take the absolute value of complex quantities, or its real part, etc.. Another common example is the evaluation of the complex-valued free energy of a metastable system, which in turn is related - via the imaginary part - with the many-body quantum transition state theory result for the reaction rate^{14,15}. As we have noted, the discussion of interaction times in Sect. 2 involves the complex-valued generalization of the classical time a particle assumes to traverse the interaction region. The traversal time t_r^{q.m.} in Eq. (14), pioneered by Sokolovski and Baskin², presents a natural quantum generalization of this classical concept. Would it not be for the Wick rotation $t \rightarrow i t$, – which is generic for the quantum dynamics – our sailing towards the tunneling time would be smooth and we readily could introduce a reasonable physical characterization of the tunneling time. The complex-valued kernel K(xtlyt_o) describing the propagation of an initial state presents us, however, with a complex-valued time-quantity, namely

$$t_{\Gamma}^{q.m.} = \int_{x_o,t_o}^{x_f,t_f} \mathcal{D} x(\bullet) t_{\Gamma}^{cl} [x(\bullet)] \exp(i/\hbar) \mathcal{S}[...] / K(x_f t_f l x_o t_o) ,$$

$$= \int \mathcal{D} x(\bullet) \int_{t_{o}}^{t_{f}} dt \int_{x_{c}}^{x_{c}} dx \, \delta \left[x - x(\bullet)\right] \exp(i \, \mathcal{S}/\hbar) \, K^{-1}(x_{f} \, t_{f} \mid x_{o} \, t_{o})$$

$$= K^{-1}(x_{f} \, t_{f} \mid x_{o} \, t_{o}) \int_{t_{o}}^{t_{f}} dt \int_{x_{c}}^{x_{c}} dx \, K(x_{f} \, t_{f} \mid x \, t) \, K(xt \mid x_{o} \, t_{o}) . \tag{17}$$

Note that Eq. (17) does not equal the "on-orbit" expression, where with $\psi_f(t_f) = \mathbb{K}(t_f|t_o)\psi_f(t_o)$

$$t_{\Gamma}^{q.m.} \neq \langle \psi_{f} | t_{\Gamma}^{cl} | \psi_{i} \rangle \langle \psi_{f} | 1 | \psi_{i} \rangle^{-1} = \int_{t_{o}}^{t_{f}} dt \int_{x_{c}}^{x_{>}} dx | \psi(xt) |^{2}$$

$$= t_{dwell time} . \qquad (18)$$

The r.h.s. equals the real-valued dwell or sojourn time discussed by various authors $^{3.9,10.13}$. In conclusion, the path integral approach does *not* supply a unique tunneling time. Both the time scales $|(\bar{t} - t_f)|$ and $|t_{\Gamma}^{q.m.}|$ present useful objects with their own purpose. They both are related – in the semiclassical limit – to the appealing result, see Eqs. (15,16), yielding the (imaginary) classical time spent for the traversal of the barrier region. Clearly, a measured tunneling time cannot be complex, and hence the results cannot be measured with a stop watch possessing complex numbers on its dial. Nevertheless, dials with such complex numbers – in clear contradistinction to Rolf Landauer's claim 16 – can exist too (see Fig. 3), and thereby do "support" the useful role of complex-valued physical objects 1,2,3,17 , such as e.g. $t_{\Gamma}^{q.m.}$.

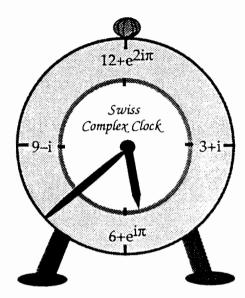


Figure 3: A clock suitable to "measure" tunneling times with complex numbers on its dial. Hereby, we used the algorithm: $t \rightarrow t + \exp[2\pi i t/t_{total}]$; i.e. hours $h \rightarrow h + \exp[2\pi i h/12]$, respectively.

In any case, it has been demonstrated here and in the literature^{1,3,13} that the hope of finding a well-defined expression for the tunneling time is erroneous. This result will be corroborated by a few further observations, expressing to some extent more closely my personal viewpoint on the issue:

- (i) First, time plays a peculiar role in quantum dynamics. The time presents within quantum theory the role of a parameter it is not an observable {B} with a corresponding Hermitean operator {B}.
- (ii) Note, that the classical traversal time for structureless particles involves a (in time) nonlocal concept i.e. no usual Schrödinger operator exists!
- (iii) The accuracy with which we can measure a duration of an event is limited by the energy time uncertainty relation

$$\Delta E \Delta t \ge \hbar/2 . \tag{19}$$

Note that generally Δt in Eq. (19) depends on the way we measure the duration. Usually, one measures the change of some observable \mathbb{L} (which does not commute with energy, and which does not exhibit an explicit time-dependence, $(\partial \mathbb{L}/\partial t)_{ex} = 0$), i.e. Δt in Eq. (19) corresponds to the quantity $\Delta t = 0$

 $\Delta L / [\frac{d}{dt} < L (t) >]$ where $\Delta L = [< L^2 > - < L >^2]^{1/2}$. Put differently, Δt measures the duration in which the expectation of L(t) changes; i.e. $< L(t) > \rightarrow < L(t) > + \Delta L$. With the uncertainty in Δt one generally finds⁸ that $\Delta E > U_b - E$, where U_b denotes the maximal barrier height. Thus, one cannot state for sure that the particle had energy $E < U_b$ and simultaneously was under the barrier.

(iv) In accordance with the energy - time uncertainty we find that $t_{\Gamma}^{q.m.}$ in Eq. (14) does not present a single fixed value but rather denotes an average. Similar conclusions have been put forward by Fertig¹⁸. Thus a definite formula which gives (at fixed energy) the traversal time in function of the transmission probability T and the phase change $\Delta \phi^{10,12,19}$ cannot be quite right. Indeed, even the evaluation of the transmission probability T within the semiclassical limit²⁰, involves multiple traversals of the barrier region corresponding to (imaginary) times, i.e.

$$t^{(n)} = i(2n+1) \tau_0$$
, $n = 0, 1, ...$ (20)

where $\tau_o = \int_{x_{-}}^{x_{-}} m \left[\hbar \kappa(x) \right]^{-1} dx$, denotes the (primitive) time-duration for traversal of the classically forbidden region (see also Reference 21). Likewise, the cumulative reaction probability²² yields with multiple periodic orbits of duration $n[2\tau_o]$, $n = 1, 2, ..., \infty$, after summation over all these multiple traversals^{22,23} of the primitive periodic orbit the well-known uniform WKB-result for the quantum transmission T(E)

$$T(E) = \left\{ 1 + \exp \Phi(E) / \hbar \right\}^{-1}$$
 (21)

Here, $\Phi(E)$, $[\Phi(E) = 2\pi (U_b - E)/\omega_b$ for an inverted parabolic barrier] denotes the Euclidean (abbreviated) bounce action at fixed energy E^{23} .

It should not go unnoted that recently several beautiful experiments have been performed to measure the tunneling time. One experiment is based directly on the macroscopic tunneling process²⁴, while other very beautiful work is based

on the close analogy between the Schrödinger equation and the microwave propagation as described by the Helmholtz equation^{25,26}. These present experimental efforts, however, neither could settle the issue of a unique "time for tunneling". At least as it concerns the experiment in Reference 24, which measures macroscopic tunneling decay in a Josephson junction shunted by a delay line, the author likes to point out the fact that the experiment did not measure any "tunneling time"; but consistently measured the decay time (lifetime) of the zero voltage state, as a function of a delay parameter t_D. This delay parameter - in turn - defines the friction mechanism, which changes as t_D is varied. Thus, the beautiful experiments in Reference 24 can be used to check different dissipative quantum decay predictions, but cannot be used in effect to substantiate an experimental verification of tunneling times²⁷.

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