Complex Interaction Times in Time-Dependent Scattering Problems.

D. SOKOLOVSKI and P. HÄNGGI

Lehrstuhl für Theoretische Physik, Universität Augsburg
Memminger Str. 6, D-8900 Augsburg, F.R.G.

Abstract. – The adiabatic criterion for a tunnelling particle interacting with an a.c. field is formulated. The adiabaticity condition is shown to involve two complex-valued time parameters, one of which is the quantum traversal time discussed recently. The two time parameters have analogues in the theory of classical Brownian motion, which guides the physical interpretation in the quantum case. Semi-classically, both parameters reduce to the conventional expression $\int mp^{-1}(x)\,dx$, representing the time of motion along the stationary classical path.

Understanding of time parameters describing the motion of a quantum particle is of great interest in such fields as potential scattering, reaction theory and quantum tunnelling. Over the years, a considerable amount of work has been invested in the problem [1-15]. However, the results of [1-15] failed to provide a unified approach to the definition of time scales for scattering problems as well as to explain the nature of different times that appear. Thus, most of the authors state the existence of various contradictory results and the problem of their classification remains open.

The purpose of this paper is, firstly, to show that the motion of a classical Brownian particle is described by a number of time parameters obtained by averaging different functionals over all the paths the particle may take. Secondly, to show that the rotation to imaginary time which allows one to obtain the Schrödinger equation from the diffusion equation leads with necessity to the existence of a corresponding number of complex time parameters in the quantum case. We illustrate this conception by formulating the adiabaticity condition for one-dimensional tunnelling also studied in [8, 10, 11]. If the motion of a particle is fast compared to the variation of an a.c. field, one can simply substitute the slow time dependence of the potential $V(x, t)$ into the static scattering amplitude. Therefore, we will specify the condition under which this substitution is justified. In the semi-classical limit, for the motion in the classically allowed region one must require that the error in the classical action be small as compared to $\hbar$. Thus, the adiabatic criterion reads: $\gamma = \hbar^{-1}\delta V\, t_{[a,b]} \ll 1$, where $t_{[a,b]} = t_b - t_a$ denotes the time the classical path $\bar{x}(t)$ spends in the interaction region $t_{a,b}$ and δV is the mean value of «perturbation» experienced by the

particle

$$\delta V = (t_b - t_a)^{-1} \int_{t_a}^{t_b} [V(\bar{x}(t), t) - V(\bar{x}(t), t_b]\, \mathrm{d}t .$$

For the case of semi-classical tunnelling, the classical path becomes complex [16]. We will show that in this case the above criterion has the same form with complex quantities $t_{[a,b]}$ and δV evaluated along this complex path. Finally, we will generalize to the full quantum case when all possible paths contribute [17]. To do so, we first investigate the classical Brownian motion.

a) Brownian motion with negative sources.

Consider a diffusion equation describing concentration of Brownian particles in the presence of absorption [18]:

$$\frac{\partial Q}{\partial t} = \frac{1}{2}\frac{\partial^2 Q}{\partial x^2} - V(x, t)\,\Theta_{[a,b]}(x)\,Q . \tag{1}$$

The function $V(x, t)$ is the probability of absorption per unit time. The sinks are localized within interval $[a, b]$. The function $\Theta_{[a,b]}(x)$ equals unity in the interval and is zero outside.

In accordance with (1), the probability density $p(x_2, t_1|x_1, t_1)$ that the particle having started its motion from x_1 at t_1 will reach x_2 at t_2 can be found by summing probabilities over all paths connecting x_1, t_1 and x_2, t_2. In particular, [18],

$$p(x_2, t_2|x_1, t_1) = \int_{x_1, t_1}^{x_2, t_2} \mathrm{D}x(t) \exp[S[x(t)]], \tag{2a}$$

$$S[x(t)] = -\int_{t_1}^{t_2} \left[\frac{\dot{x}^2}{2} + V(x, t)\,\Theta_{[a,b]}(x)\right] \mathrm{d}t . \tag{2b}$$

Associated with the path integral (2) is the averaging procedure

$$\langle F \rangle = p(x_2, t_2|x_1, t_1)^{-1} \int \mathrm{D}x(t)\, F[x(t)] \exp[S[x(t)]], \tag{3}$$

which gives the mean value $\langle F \rangle$ of the functional $F[x(t)]$ over all the paths.

Another averaging procedure connected with path integral (1) can be obtained by defining a distribution function in the part of (x, t)-plane $\{\Gamma\colon a < x < b,\ t_1 < t < t_2\}$ shown in fig. 1:

$$\mathrm{d}\mu = p(x_2, t_2|x, t)\, p(x, t|x_1, t_1) \mathrm{d}x\, \mathrm{d}t . \tag{4}$$

The corresponding mean value of arbitrary $f(x, t)$ is

$$\overline{f(x, t)} = \frac{\int\int_{\Gamma} f(x, t)\, \mathrm{d}\mu}{\int\int_{\Gamma} \mathrm{d}\mu} . \tag{5}$$

The value $f(x, t)$ enters into the numerator of (5) with a weight equal to the probability density that the particle travelling between x_1, t_1 and x_2, t_2 visits x at t.

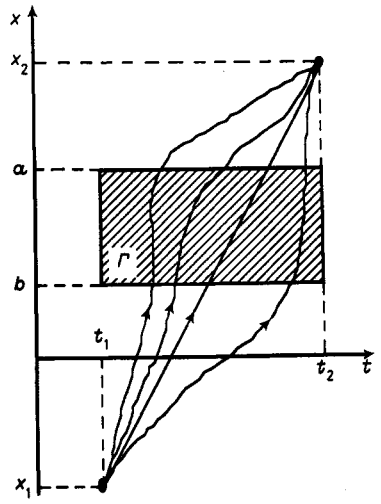

Fig. 1. – Various paths and the region Γ.

With the help of relationship $\Theta_{[a,b]}(x) = \int_a^b \delta(\lambda - x)\,\mathrm{d}\lambda$ it is readily shown that

$$\left\langle \int_{t_1}^{t_2} f(x(t), t)\,\Theta_{[a,b]}(x(t))\,\mathrm{d}t \right\rangle = \overline{f(x,t)} \left\langle \int_{t_1}^{t_2} \Theta_{[a,b]}(x(t))\,\mathrm{d}t \right\rangle. \tag{6}$$

Now we can discuss the adiabatic limit of (1), *i.e.* the conditions under which one can substitute the time-dependent function $V(x, t)$ in (1) by time-independent $V(x, t_0)$ «frozen» at some t_0 and find the accurate result for the probability density $p(x_2, t_2|x_1, t_1)$. The necessary condition is obtained by treating the difference $V(x, t) - V(x, t_0)$ as a perturbation. Thus, up to the linear terms

$$p(x_2, t_2|\,x_1, t_1)_{V(x,t)} \sim p(x_2, t_2|x_1, t_1)_{V(x,t_0)} \left\{ 1 - \left\langle \int_{t_1}^{t_2} [V(x(t), t) - V(x(t), t_0)]\,\mathrm{d}t \right\rangle_{V(x,t_0)} \right\}. \tag{7}$$

In virtue of (6), the relevant small parameter γ is seen to be

$$\gamma = \overline{(V(x,t) - V(x,t_0))} \left\langle \int_{t_1}^{t_2} \Theta_{[a,b]}(x(t))\,\mathrm{d}t \right\rangle. \tag{8}$$

The second term in the right-hand side of (8) is immediately recognized as the mean time $t_{[a,b]}(x_2, t_2|x_1, t_1)$ the particle spends in the region where the sinks are localized [18, 19]. The first term contains the information about the variation of $V(x, t)$ in time. In (8) and in the following all quantities without index $V(x, t)$ correspond to the motion in the «frozen» static $V(x, t_0)$.

b) Quantum mechanics.

One-dimensional motion of a quantum particle in the potential $V(x, t)$ is described by the

Schrödinger equation closely related to the diffusion equation (1):

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - V(x,t)\,\Theta_{[a,b]}(x)\,\Psi. \tag{9a}$$

Therefore, to define the conditions under which a quantum particle «sees» the static potential $V(x, t_0)$ we can formally repeat the arguments of the previous section by taking into account several important distinctions:

i) Expression (2) with S substituted by

$$S = \frac{i}{\hbar}\int_{t_1}^{t_2}\left[\frac{m\dot{x}(t)^2}{2} - V(x,t)\,\Theta_{[a,b]}(x)\right]\mathrm{d}t \tag{9b}$$

gives the complex probability amplitude $g(x_2, x_1, t_2, t_1)$. Correspondingly, (3) defines a «mean value» which may be complex even for a real functional F [17]. The distribution function (4), $\mathrm{d}\mu = g(x_2, x, t_2, t)\,g(x, x_1, t, t_1)\,\mathrm{d}x\,\mathrm{d}t$, is now also complex. Yet, it is natural to refer to the corresponding integrals as mean values, and we retain in the quantum case the above introduced notations $\langle F\rangle$ and $\bar{f}$.

ii) To neglect the correction to the complex static amplitude in (7) we must require that the absolute value $\left|\left\langle\int_{t_1}^{t_2}[V(x(t),t) - V(x(t),t_0)]\,\mathrm{d}t\right\rangle\right|$ is small as compared to unity.

Thus, in the quantum case the adiabaticity criterion reads:

$$\gamma = \frac{1}{\hbar}\,\overline{|(V(x,t) - V(x,t_0))|}\left|\left\langle\int_{t_1}^{t_2}\Theta_{[a,b]}(x(t))\,\mathrm{d}t\right\rangle\right| \ll 1. \tag{10}$$

It requires that the mean variation of action along all paths caused by the perturbation be negligibly small. The mean value of perturbation is multiplied by the (complex-valued) quantum traversal time $t_{[a,b]}$ whose properties have been discussed in detail in [19]. In the special case $V(x,t) = V_0\cos\omega t$, discussed in ref. [8-10], we choose t_0 equal to t_2 and expand $V(x,t) - V(x,t_2)$ up to terms linear in $t - t_2$ to obtain from (10)

$$\frac{1}{\hbar}\omega V_0\,|(\bar{t} - t_2)|\;|t_{[a,b]}(x_2, x_1, t_2 - t_1)| \ll 1. \tag{11}$$

The left-hand side contains absolute values of two time parameters of different nature: $t_{[a,b]}$ and the difference between the complex mean value $\bar{t}$ as defined by (5) and the time t_2 at which we «froze» the potential.

Of practical interest is the situation when the energy of the incident particle E is known. To fix E in (10) we assume

$$x_1 \to -\infty,\quad t_1 \to -\infty,\quad x_1/t_1 = \sqrt{\frac{2}{m}E} = \frac{\hbar k}{m}.$$

In this limit

$$\mathrm{d}\mu = g(x_2, x, t_2 - t)\,\Psi_k(x)\exp\left[-i\frac{E}{\hbar}t\right]g_0(0, x_1, -t_1)\,\mathrm{d}x\,\mathrm{d}t,$$

where $\Psi_k(x)$ is the stationary wave function describing incident flux of particles on the left side of the potential (fig. 2), and $g_0(x_2, x_1, t_2 - t_1)$ is the free-particle propagator [17, 19].

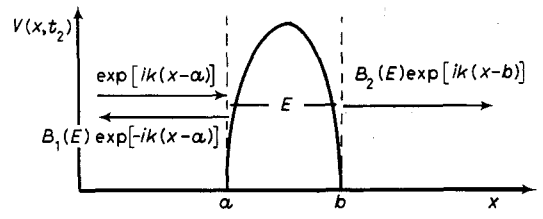

Fig. 2. – The form of the «frozen» potential $V(x, t_2)$.

Consequently, both terms in (10) depend on E and (10) becomes the condition under which the wave function of scattered particles at x_2 «follows» the variation of the potential for the case that the energy of incident particles is E. Oscillations of $d\mu$ restrict the effective region of integration in (5) to finite t's such that the particle «forgets» the form $V(x, t)$ in the distant past. For instance, for the free motion only the vicinity of the classical path (straight solid line in fig. 1) contributes to the first term in (10). It is important, however, that in general case a quantum particle can be considered fast compared to the oscillations of the potential if the absolute values $t_2 - \bar{t}(E)$ and $t_{[a,b]}(E)$ in (11) are small enough. It is easy to see that both $\bar{t}(E)$ and $t_{[a,b]}(E)$ describe the response of the scattering amplitude to a small variation of the potential in $[a, b]$ and we shall refer to them as interaction times. Thus, for the transmitted particles, $x_2 = b$, we find (the limit is taken as discussed above):

$$\bar{t}(E) = \lim \left[\int\int_\Gamma \mathrm{d}x\,\mathrm{d}t \frac{\delta g(x_2, x_1, t_2, t_1)}{\delta V(x, t)} \right]^{-1} \int\int_\Gamma \mathrm{d}x\,\mathrm{d}t\, t \frac{\delta g(x_2, x_1, t_2, t_1)}{\delta V(x, t)} =$$

$$= t_2 + i\hbar \frac{\partial}{\partial E_1} \ln F(E, E_1)|_{E_1 = E}, \qquad (12a)$$

$$t_{[a,b]}(E) = i\hbar \lim \int\int_\Gamma \mathrm{d}x\,\mathrm{d}t \frac{\delta \ln g(x_2, x_1, t_2, t_1)}{\delta V(x, t)} = F(E, E_1)|_{E_1 = E}, \qquad (12b)$$

where

$$F(E, E_1) = im\hbar^{-1} k(E_1)^{-1} \left\{ \frac{B_2(E) - B_2(E_1)}{k(E_1) - k(E)} + \frac{B_2(E_1)}{B_2^*(E_1)} \frac{(B_1^*(E_1) B_2(E) - B_1(E) B_2^*(E_1))}{k(E_1) + k(E)} \right\}.$$

Here $B_{1,2}(E)$ are the scattering amplitudes shown in fig. 2. Semi-classically, (12a) and (12b) reduce to the familiar expressions

$$\frac{1}{2} \int_a^b \frac{m\mathrm{d}x}{p} \quad \text{and} \quad \int_a^b \frac{m\mathrm{d}x}{p}$$

($p = |(2m(E - V))^{1/2}|$ if $E > V$, $i|(2m(E - V))^{1/2}|$ otherwise), evaluated along the classical path.

Finally, we discuss the result of [8, 10], where a small perturbation $W \cos \omega t$ has been added to a rectangular barrier within the barrier region. The square of the tunnelling time,

τ^2, has been defined as the ratio between the probability of absorbtion of a quantum $\hbar\omega$ as $\omega \to 0$ and the factor of $(W/2\hbar)^2|B_2|^2$. In this case the wave function of transmitted particles has the form

$$\Psi(x,t) = B_2(E)\exp[-iEt + ik(x-b)]\cdot$$

$$\cdot\left\{1 + \frac{W}{\hbar}[\cos\omega t - \omega(t-\bar{t}(E))\sin\omega t + \ldots]\, t_{[a,b]}(E) + O(W^2)\right\}. \qquad (13)$$

Thus, in the approach of [10], τ becomes equal to $|t_{[a,b]}|$. However, τ is not the time which compares to ω in the low-frequency limit of (13). This limit is reached if $\omega|t-\bar{t}(E)| \ll 1$. Note that $t-\bar{t}(E)$ and $t_{[a,b]}(E)$ are of the same order in the semi-classical limit (*i.e.* for opaque rectangular barriers) but may strongly differ in the full quantum case.

In conclusion: it is shown that the condition for adiabatic interaction of a quantum particle with an applied a.c. field involves two complex interaction times of different nature. Both of them are most simply related to the time parameters describing the motion of a classical Brownian particle. Both times are complex and from the way we obtained their expressions it is clear that the complexity of time parameters is an inherent property of the quantal motion. Thus, in general it is unlikely that any physical meaning can be ascribed to their real and imaginary parts separately.

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