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Time as a Quantum Observable, Canonically Conjugated to Energy, and Time-Dependent Analysis of Quantum Processes

V.S.Olkhovsky

Institute for Nuclear Research of NASU, Kiev, Ukraine

olkhovsk@kinr.kiev.ua, olkhovsky@mail.ru

ABSTRACT

The review of the author papers and also of papers of the other authors is presented time in quantum mechanics and quantum electrodynamics as an observable, canonically conjugate to energy. This report deals with the maximal hermitian (but non-self-adjoint) operator for time which appears for systems with continuous energy spectra. Two measures of averaging over time and connection between them are analyzed. The results of the study of time as a quantum observable in the cases of the discrete energy spectra are also presented, and in this case the quasi-self-adjoint time operator appears. Then some applications of time analysis of quantum processes are shortly reviewed.

Keywords: *time, maximal hermitian operator, continuous energy spectrum, discrete energy spectrum, time-energy indeterminacy relation, time analysis of tunneling processes.*

1. INTRODUCTION

During almost ninety years (see, for example, [1]) it is known that time cannot be represented by a self-adjoint operator, with the possible exception of special abstract systems (such as an electrically charged particle in an infinite uniform electric field and a system with the limited from both below and above energy spectrum). This fact results to be in contrast with the known circumstance that time, as well as space, in some cases plays the role just of a parameter, while in some other cases *is* a physical observable which *ought* to be represented by an operator. The list of papers devoted to the problem of time in quantum mechanics is extremely large (see, for instance, [2-38], and references therein). The same situation had to be faced also in quantum electrodynamics and, more in general, in relativistic quantum field theory (see, for instance, [9,34,37,38]).

As to quantum mechanics, the first set of known and cited articles is [2-13]. The second set of papers on time as an observable in quantum physics [14-37] appeared from the end of the eighties and chiefly in the nineties and more recently, stimulated mainly by the need of a self-consistent definition for collision duration and tunneling time. It is noticeable that many of this second set of papers appeared however to ignore the Naimark theorem from [39], which had previously constituted an important basis for the results in refs.[10-13]. This Naimark theorem states [39] that the non-orthogonal spectral decomposition $E(\lambda)$ of a hermitian operator H is of the Carleman type (which is unique for the maximal hermitian operator), i.e. it *can be approximated* by a succession of the self-adjoint operators, the spectral functions of which do weakly converge to the spectral function $E(\lambda)$ of the operator H .

Namely, by exploiting that Naimark theorem, it has been shown by V.S.Olkhovsky and E.Recami [10,11,13] (more details having been added in [14-16,21,22,34,37]) and, independently, by A.S.Holevo [12] that, for systems with continuous energy spectra, time can be introduced as a quantum-mechanical observable,

canonically conjugate to energy. More precisely, the time operator resulted to be maximal hermitian, even if not self-adjoint. Then, in [15 (ref.1), 22(ref.3), 37] it was clarified that time can be introduced also for these systems as a quantum-mechanical observable, canonically conjugate to energy, and the time operator resulted to be quasi-self-adjoint (more precisely, it can be chosen as an almost self-adjoint operator with practically almost any degree of the accuracy).

Now let us analyse the so-called *positive-operator-value-measure* (POVM) approach, often used in the second set of papers on time in quantum physics (for instance, in [17-20,23-33,35,36]). This approach, in general, is well-known in the various approaches to the quantum theory of measurements approximately from the sixties and had been applied in the simplest form for the time-operator problem in the case of the free motion already in [40]. Then, in [17-20,23-33,35,36] (often with certain simplifications and abbreviations) it was affirmed that the generalized decomposition of unity (or POV measures) is reproduced from any self-adjoint extension of the time operator into the space of the extended Hilbert space (usually, with negative values of energy E in the left semi-axis) citing the Naimark's dilation theorem from [41]. However, it was realized factually only for the simple cases like the particle free motion. As to our approach, it is based on *another* Naimark's theorem (from [39]), cited above, and *without* any extension of the physical Hilbert space of usual wave functions (wave packets) with the subsequent return projection to the previous space of wave functions; and, moreover, it had been published in [9-11,13] (and independently in the papers of A.S.Holevo [12], with the same principal idea) much earlier than [17-20,23-33,35,36]. Being based on the earlier published remarkable Naimark theorem [39] and on the general known mathematical foundations of [42,43], it is *much more direct, simple and general, and at the same time mathematically not less rigorous* than POVM approach!

1. Time as a quantum observable and general definitions of mean times and mean durations of quantum processes for systems with continuous energy

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spectra. For systems with continuous energy spectra, the energy, can be introduced for time: following simple operator, canonically conjugate to

$$\hat{t} = \begin{cases} t & \text{in the (time) } t\text{-representation,} \\ \end{cases} \quad (1a)$$

$$\begin{cases} -i\hbar \frac{\partial}{\partial E} & \text{in the (energy) } E\text{-representation} \end{cases} \quad (1b)$$

which is not self-adjoint, but is *hermitian*, and acts on square-integrable space-time wavepackets in representation (1a), and on their Fourier-transforms in representation (1b), once the point $E=0$ is eliminated (i.e., once one deals only with moving packets, i.e., excludes any *non-moving* back tails, as well as, of course, the zero flux cases). Such a condition is enough for operator (1a,b) to be a “*maximal hermitian*” operator [10-13] (see also [16,22,38,39]), according to Akhiezer & Glazman’s terminology [42]. The elimination of the

point $E=0$ is not restrictive since the “rest” states with the zero velocity, the wave-packets with *non-moving* rear tails, and the wave-packets with zero flux are unobservable. Then all unphysical negative values of energy E are excluded since for a free particle all physical values of kinetic energy are positive.

Operator (1b) is defined as acting on the space P of the continuous, differentiable, square-integrable functions $f(E)$ that satisfy the conditions.

$$\int_0^\infty |f(E)|^2 dE < \infty; \int_0^\infty |\partial f(E) / \partial E|^2 dE < \infty; \int_0^\infty |f(E)|^2 E^2 dE < \infty, \quad (2)$$

and the condition

$$f(0) = 0 \quad (3)$$

which is a space P dense in the Hilbert space of L^2 functions defined (only) over the semi-axis $0 \leq E < \infty$. Obviously, the operator (1a,b) is hermitian, i.e. the relation $(f_1, \hat{t} f_2) = ((\hat{t} f_1), f_2)$ holds, only if all square-integrable functions $f(E)$ in the space on which it is defined vanish for $E=0$.

Operator \hat{t} has no hermitian extension because otherwise one could find at least one function $f_0(E)$ which satisfies the condition $f_0(0) \neq 0$ but that is inconsistent with the propriety of being hermitian. So, according to [39, 42], \hat{t} is a maximal hermitian operator.

Essentially because of these reasons, earlier Pauli (see, for instance, [1]) rejected the use of a time operator: and

$$W(x,t)dt = \frac{j(x,t)dt}{\int_{-\infty}^{\infty} j(x,t)dt}, \quad (4)$$

where the probabilistic interpretation of $j(x,t)$ (namely in *time*) corresponds to the flux probability density of a particle passing through point x at time t (more precisely, passing through x during a unit time interval centered at t), when travelling in the positive x -

this had the result of practically stopping studies on this subject for about forty years. However, as far back as in [43] von Neumann had claimed that considering in quantum mechanics only self-adjoint operators could be too restrictive.

In order to consider *time as an observable in quantum mechanics* and to define the observable mean times and durations, one needs to introduce not only the time operator, but also, in a self-consistent way, the measure (or weight) of averaging over time. In the simple one-dimensional (1D) and one-directional motion such *measure* (weight) can be obtained by the simple quantity:

direction.. Such a measure had not been postulated, but is just a direct consequence of the well-known probabilistic (*spatial*) interpretation of $\rho(x,t)$ and of the continuity relation.

$$\partial \rho(x,t) / \partial t + \text{div } j(x,t) = 0 \quad (5)$$

for particle motion in the field of any hamiltonian in the description of the 1D Schroedinger equation. Quantity $\rho(x,t)$ is the probability of finding a moving particle

inside a unit space interval, centered at point x , at time t . The probability density $\rho(x,t)$ and the flux probability-density $j(x,t)$ are related with the wave function $\Psi(x,t)$

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by the usual definitions $\rho(x,t)=|\Psi(x,t)|^2$ and $j(x,t) = \text{Re} [\Psi^*(x,t) (\hbar/i\mu) \partial\Psi(x,t)/\partial x]$. The measure (4) was firstly investigated in [13,15,16,21,22].

When the flux density $j(x,t)$ changes its sign, the quantity $W(x,t)dt$ is no longer positive definite and it

acquires a physical meaning of a probability density *only* during those partial time-intervals in which the flux density $j(x,t)$ does keep its sign. Therefore, let us introduce the two measures, by separating the positive and the negative flux-direction values (i.e., flux signs):

$$W_{\pm}(x,t)dt = \frac{j_{\pm}(x,t)dt}{\int_{-\infty}^{\infty} j_{\pm}(x,t)dt} \tag{4a}$$

with $j_{\pm}(x,t)=j(x,t)\Theta(\pm j)$ where $\Theta(z)$ is the Heaviside step function. It had been made firstly in [16,21,22]. Actually, one can rewrite the continuity relation (5) for

$$\frac{\partial\rho_{>}(x,t)}{\partial t} = -\frac{\partial j_{+}(x,t)}{\partial x} \quad \text{and} \quad \frac{\partial\rho_{<}(x,t)}{\partial t} = -\frac{\partial j_{-}(x,t)}{\partial x} , \tag{6}$$

respectively.

Then, one can eventually define the mean value $\langle t(x) \rangle$ of the time t at which a particle passes through position x (when travelling in only one positive

those time intervals, for which $j = j_{+}$ or $j = j_{-}$ as follows:

x -direction), and $\langle t_{\pm}(x) \rangle$ of the time t at which a particle passes through position x , when travelling in the positive or negative direction, respectively

$$\langle t(x) \rangle = \frac{\int_{-\infty}^{\infty} tj(x,t)dt}{\int_{-\infty}^{\infty} j(x,t)dt} = \frac{\int_0^{\infty} dE \frac{1}{2} [G^*(x,E)\hat{t}vG(x,E) + vG^*(x,E)\hat{t}G(x,E)]}{\int_0^{\infty} dEv|G(x,E)|^2} \tag{7a}$$

where $G(x,E)$ is the Fourier-transform of the moving one-dimensional (1D) wave packet

$$\Psi(x,t) = \int_0^{\infty} G(x,E)\exp(-iEt/\hbar) dE = \int_0^{\infty} g(E)\varphi(x,E)\exp(-iEt/\hbar)dE \tag{8}$$

when going on from the time representation to the energy one,

$$\langle t_{\pm}(x) \rangle = \frac{\int_{-\infty}^{\infty} tj_{\pm}(x,t)dt}{\int_{-\infty}^{\infty} j_{\pm}(x,t)dt} , \tag{7b}$$

and also the mean durations of particle 1D transmission from x_i to $x_f > x_i$ and 1D particle reflection from the region (x_i, ∞) into $x_f \leq x_i$:

$$\langle \tau_T(x_i, x_f) \rangle = \langle t_{+}(x_f) \rangle - \langle t_{+}(x_i) \rangle \quad \text{and} \quad \langle \tau_R(x_i, x_f) \rangle = \langle t_{-}(x_f) \rangle - \langle t_{+}(x_i) \rangle , \tag{7c}$$

respectively. Of course, it is possible to pass in eq. (7b)

also to integrals $\int dE\dots$, similarly to (7a) by using the

unique Fourier (Laplace) - transformations and the

energy expansion of $j_{\pm}(x,t)=j(x,t)\Theta(\pm j)$, but it is evident that they result to be rather bulky. The three-dimensional case can be similarly analyzed ([13,15,38]).

Now, one can see that two canonically conjugate operators, the time operator (1) and the energy operator

$$\hat{E} = \begin{cases} E & \text{in the energy (E-) representation,} \\ i\hbar \frac{\partial}{\partial t} & \text{in the time (t-) representation,} \end{cases} \quad (9)$$

satisfy the typical commutation relation

$$[\hat{E}, \hat{t}] = i\hbar. \quad (10)$$

Although up to now according to the Stone and von Neumann theorem [44] the relation (10) has been interpreted as holding *only* for the pair of the self-adjoint canonically conjugate operators, in both representations, and it was not directly generalized for *maximal hermitian operators*, the difficulty of such direct generalization has in fact been by-passed by

introducing \hat{t} with the help of the *single-valued* Fourier(Laplace)-transformation from the t -axis ($-\infty < t < \infty$) to the E -semi-axis ($0 < E < \infty$) and by utilizing the peculiar mathematical properties of maximal symmetric operators (as in [12,13,15,22,37,38]), described in detail, e.g., in [42].

Actually, from eq.(16) the uncertainty relation

$$\Delta E \Delta t \geq \hbar/2 \quad (11)$$

where the standard deviations are $\Delta a = \sqrt{Da}$, quantity Da being the variance $Da = \langle a^2 \rangle - \langle a \rangle^2$; and $a = E, t$, while $\langle \dots \rangle$ denotes an average over t by the measures $W(x,t)dt$ or $W_{\pm}(x,t)dt$ in the t -representation or an average over E similar to the right-hand-part of (7a) and (8) in the E -representation) was derived by the simple generalizing of the similar procedures which are standard in the case of self-adjoint canonically conjugate quantities (see [11-13,15,22,37,38]). Moreover, relation (10) satisfies the Dirac "correspondence principle", since the classical Poisson brackets $\{q_0, p_0\}$, with $q_0 = t$ and $p_0 = -E$, are equal to unity [45]. In [13] (see also [15]) it was also shown that *the differences* between the mean times at which a wave-packet passes through a *pair* of points obey the Ehrenfest correspondence principle; in other words, in [13,15] the Ehrenfest theorem was suitably generalized.

After what precedes, one can state that, for systems with continuous energy spectra, the mathematical properties of the maximal hermitian operators (described, in particular, in [36,39]), like \hat{t} in eq.(1), are *sufficient* for considering them as quantum observables: Namely, the *uniqueness* of the "spectral decomposition" (also called spectral function) for operators \hat{t} , as well as for \hat{t}^n ($n > 1$) guarantees

(although such an expansion is not orthogonal) the *equivalence* of the mean values of any analytic functions of time, evaluated either in the t - or in the E -representations. In other words, the existence of this expansion is equivalent to a *completeness relation* for the (formal) eigenfunctions of \hat{t}^n ($n > 1$), corresponding with any accuracy to *real eigenvalues* of the continuous spectrum; such eigenfunctions belonging to the space of the square-integrable functions of the energy E with the boundary conditions (2)-(3).

From this point of view, there is *no practical difference between self-adjoint and maximal hermitian operators* for systems with continuous energy spectra. Let us underline that the *mathematical* properties of \hat{t}^n ($n > 1$) are quite enough for considering *time* as a *quantum-mechanical observable* (like for energy, momentum, spatial coordinates,...) *without having to introduce any new physical postulates*.

2. Time as an observable and time-energy uncertainty relation for quantum-mechanical systems with discrete energy spectra.

For systems with discrete energy spectra it is natural (following [15,37]) to introduce wave packets of the form

$$\psi(x,t) = \sum_{n=0}^{\infty} g_n \varphi_n(x) \exp[-i(\varepsilon_n - \varepsilon_0)t/\hbar] \quad (12)$$

(where $\varphi_n(x)$ are orthogonal and normalized wave functions of system bound states which satisfy equation $\hat{H} \varphi_n(x) = \varepsilon_n \varphi_n(x)$, \hat{H} being the system Hamiltonian;

$\sum_{n=0}^{\infty} |g_n|^2 = 1$; here we factually omitted a non-

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significant phase factor $\exp(-i\varepsilon_0 t/\hbar)$ as being general for all terms of the sum $\sum_{n=0}^{\infty}$) for describing the evolution of systems in the regions of the purely discrete spectrum. Without limiting the generality, we choose moment $t=0$ as an initial time instant.

Firstly, we shall consider those systems, whose energy levels are spaced with distances for which the maximal common divisor is *factually existing*. Examples of such systems are *harmonic oscillator, particle in a rigid box and spherical spinning top*. For these systems the wave packet (12) is a periodic function of time with the period (*Poincaré cycle time*) $T = 2\pi\hbar/D$, D being the

maximal common divisor of distances between system energy level.

In the t -representation the relevant energy operator \hat{H} is a self-adjoint operator acting in the space of *periodical* functions whereas the function $t\psi(t)$ does not belong to the same space. In the space of periodical functions the time operator \hat{t} , even in the eigen representation, has to be also a periodical function of time t . This situation is quite similar to the case of azimuth angle φ which is canonically conjugated to angular momentum \hat{L}_z (see, for instance, [46,47]). Utilizing the example and result from [48], let us choose, instead of t , a *periodical* function

$$\hat{t} = t - T \sum_{n=0}^{\infty} \Theta(t - [2n+1]T/2) + T \sum_{n=0}^{\infty} \Theta(-t - [2n+1]T/2) \tag{13}$$

which is the so-called saw-function of t (see Fig.1).

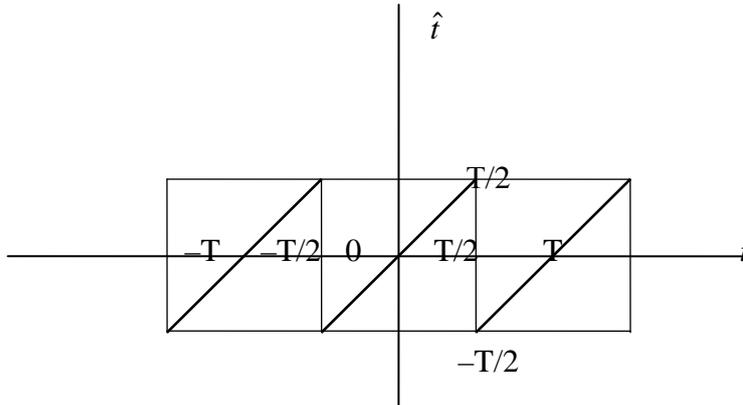


Fig.1. The periodical saw-tooth function for time operator for the case of (13).

This choice is convenient because the periodical function of time operator (13) is linear function (one-directional) within each Poincaré interval, i.e. time conserves its flowing and its usual meaning of an *order* parameter for the system evolution.

The commutation relation of the *self-adjoint* energy and time operators acquires in this case (discrete energies and periodical functions) the form:

$$[\hat{E}, \hat{t}] = i\hbar \{1 - T \sum_{n=0}^{\infty} \delta(t - [2n+1]T)\}. \tag{14}$$

Let us recall (see, e.g. [48]) that a generalized form of uncertainty relation holds

$$(\Delta A)^2 \cdot (\Delta B)^2 \geq \hbar^2 [\langle N \rangle]^2 \tag{15}$$

for two self-adjoint operators \hat{A} and \hat{B} , canonically conjugate each to other by the commutator

$$[\hat{A}, \hat{B}] = i\hbar \hat{N}, \tag{16}$$

\hat{N} being a third self-adjoint operator. One can easily obtain

$$(\Delta E)^2 \cdot (\Delta t)^2 \geq \hbar^2 \left[1 - \frac{T |\psi(T/2 + \gamma)|^2}{\int_{-T/2}^{+T/2} |\psi(t)|^2 dt} \right], \quad (17)$$

where the parameter γ (with an arbitrary value between $-T/2$ and $+T/2$) is introduced for the univocality of calculating the integral on right part of (17) over dt in the limits from $-T/2$ to $+T/2$, just similarly to the procedure introduced in [46] (see also [48]).

From (17) it follows that when $\Delta E \rightarrow 0$ (i.e. when $|g_n| \rightarrow \delta_{mn}$) the right part of (17) tends to zero since $|\psi(t)|^2$ tends to a constant. In this case the distribution of time instants of wave-packet passing through point x in the limits of one Poincaré cycle becomes uniform.

In principle, one can obtain the expression for the time operator (13) also in energy representation.

In general cases, for excited states of nuclei, atoms and molecules, *level distances in discrete spectra have not strictly defined the maximal common divisor and hence they have not the strictly defined time of the Poincaré cycle*. And also there is no strictly defined passage from the discrete part of the spectrum to the continuous part. Nevertheless, even for those systems one can introduce an approximate description (and with any desired degree of the accuracy within the chosen maximal limit of the level width, let us say, γ_{lim}) by

In the degenerate case when at the state (12) the sum $\sum_{n=0}^{\infty}$ contains only one term ($g_n \rightarrow \delta_{mn}$), the evolution is absent and the time of the Poincaré cycle is equal formally to infinity.

3. Time analysis of quantum processes, based on the application of time as a quantum observable

(1) Time analysis of various propagations for non-relativistic particles and photons revealed not only the similarity for non-relativistic-particle and photon propagating [51-53] but also permitted to introduce the maximal hermitian operator of time also for quantum electrodynamics (at least, for one-dimensional photon propagations) [34,37,38].

(2) There are known two measures of averaging on time in quantum mechanics. Earlier it was exposed a measure of averaging on passing (motion) of a particle or of a photon. The second measure characterizes the accumulation or dwelling (or sojourning) of particles or photons in the limited space volume during their passing through it.

(3) *Time analysis of tunneling processes:*

(a) Actually, the time operator (1) has been rather fruitfully used in the case of the tunneling times (see refs [16,21,22,34]). We have established that practically all earlier known particular tunneling times appear to be the special cases of the mean tunneling time or of the square root of the variance in the tunneling-time distribution (or pass into them under some boundary conditions),

When $\Delta E \gg D$ and $|\psi(T+\gamma)|^2 \ll T \int_{-T/2}^{T/2} |\psi(t)|^2 dt$, the periodicity condition may be

inessential for $\Delta t \ll T$, i.e. (17) passes to uncertainty relation (7), which is just the same one as for systems with continuous spectra.

quasi-cycles with quasi-periodical evolution and for sufficiently long intervals of time the motion inside such systems (however, less than \hbar/γ_{lim}) one can consider as a *periodical motion also with any desired accuracy*. For them one can choose (define) a time of the Poincaré cycle with any desired accuracy, including in one cycle as many quasi-cycles as it is necessary for demanded accuracy. Then, with the same accuracy the *quasi-self-adjoint time operator* (31) or (36) can be introduced and all time characteristics can be defined.

If a system has both (continuous and discrete) regions of the energy spectrum, one can easily use the forms (1) for the continuous energy spectrum and the forms (13) for the discrete energy spectrum.

defined within the general O-R approach. It had been carried out in some reviews also the connection of other earlier known approaches or simultaneously elaborated approaches with the O-R approach which had been recognized as the most self-consistent definition of the tunnelling time within the conventional quantum mechanics (see, for instance, [54]).

(b) Although there is no classical limit for particle motions inside potential barriers in the case of sub-barrier kinetic energies, there are nonzero probability density and nonzero probability flux density inside such barriers due to the particle wave properties. It is meaningful to stress also that, although any direct classical limit for particle tunnelling through potential barrier with sub-barrier energies is really absent, *there is the direct classical limit for wave-packet tunneling*. Let us recall *real evanescent and anti-evanescent waves*, well-known in *classical optics* and in *classical acoustics* (see, for instance, [37,38, 55,56]).

(c) As a result of the interference between these evanescent and anti-evanescent waves, an essentially non-uniform behavior of the wave-packet motion [16,34].

(d) Moreover, there is an infinite series of *multiple internal reflections of evanescent and anti-evanescent waves* from both entrance and exit barrier walls inside the barrier [13].

(e) The Hartman “saturation” effect was revealed and analyzed (see, for instance, [16,34]). It consists in the independency of tunneling times from the barrier width for large (opaque) barriers both for total exit peaks and also for every peak portion outwards from a barrier during any step of multiple internal reflections. In the case of total exit peak outwards from the back barrier wall this was confirmed experimentally for electromagnetic (microwave) tunneling in [58-60].

(f) For wide momentum spreads in the initial wave packets there were theoretically revealed the strong violations of the Hartman effect – namely the decreasing of tunneling times with increasing of barrier widths (sometimes up to the negative values) [61].

(g) As it was shown in [56,62], the non-stationary fluxes, corresponding to the wave packets of only evanescent or only anti-evanescent waves separately, describe oscillations which *appear instantaneously in all space inside a barrier*. It is true for both photons (in one-dimensional quantum electrodynamics) and non-relativistic particles [38,56,62]. Such a phenomenon means a manifestation of (a) the influence of *a barrier as a whole* on the tunneling particles and photons, and hence, of (b) the *non-local* behavior of tunneling particles and photons with sub-barrier energies inside

barriers (see, for instance, Appendix A of ref. [38,56,62]).

It is rather curious that applying various mathematical methods (virtual-momentum (but with *real* values) Fourier-expansion, instanton approach over the imaginary time axis etc) one can describe such wave packets as *current* wave packets in various exotic spaces with unusual metrics [19-21].

The Hartman effect (HE) is now extended for all expressions of mean tunneling times, however, with sufficiently narrow momentum spreads of initial particle wave packets (and, of course, for quasi-monochromatical particles). The violations of the HE are revealed and explained for the presence of the absorption and also for the cases of the rather large momentum spreads of initial particle wave packets.

It is rather interesting and perspective to develop the time analysis of the whole-universe tunnelling through the barrier of the quantum gravitation curve during the initial Big-Bang inflation period, starting from the Hamiltonian approach to time operator (see, for instance, [8,37,38]), *defined by the operator equation*

$$[H, T] = i\hbar,$$

and, using then the dual equations $H\Psi = i\hbar\partial\Psi/\partial t$ and

$$T\Phi = -i\hbar \frac{\partial}{\partial E} \Phi, \quad \Phi \text{ being the Fourier-component of}$$

$$\Psi = \int_0^\infty dt e^{-iEt/\hbar} \Phi(E).$$

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