

# Time as Quantum Observable, Canonical Conjugated to Energy

Vladislav S. Olkhovsky<sup>1</sup>, Erasmo Recami<sup>2</sup> and Sergei P. Maydanyuk<sup>3</sup>

<sup>1</sup>*Institute for Nuclear Research, National Academy of Sciences*

<sup>2</sup>*Facoltà di Ingegneria, Università statale di Bergamo, Bergamo  
and INFN-Sezione di Milano, Milan*

<sup>3</sup>*Institute for Nuclear Research, National Academy of Sciences  
<sup>1,3</sup>Ukraine  
<sup>2</sup>Italy*

## 1. Introduction

Time, as well as 3-position, sometimes is a parameter, but sometimes is an observable that in quantum theory would be expected to be associated with an operator. However, almost from the birth of quantum mechanics (cf., e.g., Ref.(Pauli, 1926; 1980)), it is known that time cannot be represented by a selfadjoint operator, except in the case of special systems (such as an electrically charged particle in an infinite uniform electric field)<sup>1</sup>. The list of papers devoted to the problem of time in quantum mechanics is extremely large (see, for instance, Refs. (Aharonov et al., 1998; Atmanspacher & Amann, 1998; Blanchard P & Jadczyk, 1996; Busch et al., 1994; Delgado, 1999; Egusquiza & Muga, 1999; Giannitrapani, 1997; Gózdź A & Dębicki, 2007; Grot et al., 1996; Holevo, 1978; 1982; Kijowski, 1997; Kobe et al., 1994; Kochański & Wo'dkievicz, 1999; Leo'n, 1997; Muga et al., 1999; Olkhovsky & Recami, 1968; 1969; 1970; Olkhovsky, 1973; Olkhovsky et al., 1974; Olkhovsky, 1984; 1990; 1992; Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky, 1998; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007; Olkhovsky, 2009; 2011; Recami, 1976; 1977; Srinivas & Vijayalakshmi, 1981; Toller, 1999; Wang & Xiong, 2007), 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, Refs.(Olkhovsky & Recami, 1968; 1969; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007)).

As to quantum mechanics, the very first relevant articles are probably Refs. (Holevo, 1978; 1982; Olkhovsky & Recami, 1968; 1969; 1970; Olkhovsky, 1973; Olkhovsky et al., 1974; Olkhovsky, 1984; 1990; 1992; 1998; Recami, 1976; 1977), and refs. therein. A second set of papers on time in quantum physics (Aharonov et al., 1998; Atmanspacher & Amann, 1998; Blanchard P & Jadczyk, 1996; Busch et al., 1994; Delgado, 1999; Egusquiza & Muga, 1999; Giannitrapani, 1997; Gózdź A & Dębicki, 2007; Grot et al., 1996; Kijowski, 1997; Kobe et al.,

<sup>1</sup> This is a consequence of the semi-boundedness of the continuous energy spectra from below (usually from zero). Only for an electrically charged particle in an infinite uniform electric field, and other very rare special systems, the continuous energy spectrum is not bounded and extends over the whole axis from  $-\infty$  to  $+\infty$ . It is curious that for systems with continuous energy spectra bounded from above and from below, the time operator is however selfadjoint and yields a discrete time spectrum.

1994; Kochański & Wo'dkiewicz, 1999; Leo'n, 1997; Muga et al., 1999; Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007; Srinivas & Vijayalakshmi, 1981; Toller, 1999; Wang & Xiong, 2007) appeared in the nineties, stimulated partially by the need of a consistent definition for the tunneling time. It is noticeable, and let us stress it right now, that this second set of papers seems however to have ignored Naimark's theorem (Naimark, 1940), which had previously constituted (directly or indirectly) an important basis for the results in Refs. (Holevo, 1978; 1982; Olkhovsky & Recami, 1968; 1969; 1970; Olkhovsky, 1973; Olkhovsky et al., 1974; Olkhovsky, 1984; 1990; 1992; 1998; Recami, 1976; 1977), moreover, all the papers (Aharonov et al., 1998; Atmanspacher & Amann, 1998; Blanchard P & Jadczyk, 1996; Busch et al., 1994; Grot et al., 1996; Kobe et al., 1994; Leo'n, 1997; Srinivas & Vijayalakshmi, 1981) attempted at solving the problem of time as a quantum observable by means of formal mathematical operations performed *outside* the usual Hilbert space of conventional quantum mechanics. Let us recall that Naimark's theorem states (Naimark, 1940) that the non-orthogonal spectral decomposition of a hermitian operator *can be approximated* by an orthogonal spectral function (which corresponds to a selfadjoint operator), in a weak convergence, *with any desired accuracy*.

The main goal of the first part of the present paper is to justify the use of time as a quantum observable, basing ourselves on the properties of the hermitian (or, rather, maximal hermitian) operators for the case of continuous energy spectra: cf., e.g., the Refs. (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; 2004; Olkhovsky & Recami, 2007)).

The question of time as a quantum-theoretical observable is conceptually connected with the much more general problem of the four-position operator and of the canonically conjugate four-momentum operator, both endowed with an hermitian and an anti-hermitian part, for relativistic spin-zero particles: This problem is analyzed in the second part of the present paper.

In the third part of this work, it is shown how non-hermitian operators can be meaningfully and extensively used, for instance, for describing *unstable states* (decaying resonances). Brief mentions are added of the cases of quantum dissipation, and of the nuclear optical potential.

## **2. Time operator in non-relativistic quantum mechanics and in quantum electrodynamics**

### **2.1 On *Time* as an observable in non-relativistic quantum mechanics for systems with continuous energy spectra**

The last part of the above-mentioned list (Aharonov et al., 1998; Atmanspacher & Amann, 1998; Blanchard P & Jadczyk, 1996; Busch et al., 1994; Delgado, 1999; Egusquiza & Muga, 1999; Giannitrapani, 1997; Gózdź A & Dębicki, 2007; Grot et al., 1996; Kijowski, 1997; Kobe et al., 1994; Kochański & Wo'dkiewicz, 1999; Leo'n, 1997; Muga et al., 1999; Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007; Toller, 1999; Wang & Xiong, 2007), of papers, in particular Refs. (Aharonov et al., 1998; Atmanspacher & Amann, 1998; Blanchard P & Jadczyk, 1996; Delgado, 1999; Egusquiza & Muga, 1999; Giannitrapani, 1997; Gózdź A & Dębicki, 2007; Grot et al., 1996; Kijowski, 1997; Kobe et al., 1994; Kochański & Wo'dkiewicz, 1999; Leo'n, 1997; Muga et al., 1999; Toller, 1999; Wang & Xiong, 2007), appeared in the nineties, devoted to the problem of Time in non-relativistic quantum mechanics, essentially because of the need to define the tunnelling

time. As remarked, those papers did not refer to the Naimark theorem<sup>2</sup> (Naimark, 1940) which had mathematically supported, on the contrary, the results in (Holevo, 1978; 1982; Olkhovsky & Recami, 1968; 1969; 1970; Olkhovsky, 1973; Olkhovsky et al., 1974; Olkhovsky, 1984; 1990; 1992; 1998; Recami, 1976; 1977), and afterwards in (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007). Indeed, already in the seventies (in Refs. (Olkhovsky & Recami, 1968; 1969; 1970; Olkhovsky, 1973; Olkhovsky et al., 1974; Recami, 1976; 1977) while more detailed presentations and reviews can be found in (Olkhovsky, 1984; 1990; 1992; 1998) and independently in (Holevo, 1978; 1982)), it was proven that, for systems with continuous energy spectra, Time is a quantum-mechanical observable, canonically conjugate to energy. Namely, it had been shown the time operator

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

to be not selfadjoint, but hermitian, and to act on square-integrable space-time wave packets in the representation (1a), and on their Fourier-transforms in (1b), once point  $E = 0$  is eliminated (i. e., once one deals only with moving packets, excluding any *non-moving* rear tails and the cases with zero fluxes)<sup>3</sup> In Refs.(Olkhovsky, 1984; 1990; 1992; 1998) and (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007), the operator  $\hat{t}$  (in the  $t$ -representation) had the property that any averages over time, in the one-dimensional (1D) scalar case, were to be obtained by use of the following *measure* (or weight):

$$W(t, x) dt = \frac{j(x, t) dt}{\int_{-\infty}^{+\infty} j(x, t) dt}, \quad (2)$$

where the the flux density  $j(x, t)$  corresponds to the (temporal) probability for a particle to pass through point  $x$  during the unit time centered at  $t$ , when traveling in the positive  $x$ -direction. Such a measure is not postulated, but is a direct consequence of the well-known probabilistic *spatial* interpretation of  $\rho(x, t)$  and of the continuity relation  $\partial\rho(x, t)/\partial t + \text{div}j(x, t) = 0$ . Quantity  $\rho(x, t)$  is, as usual, the probability of finding the considered moving particle inside a unit space interval, centered at point  $x$ , at time  $t$ .

Quantities  $\rho(x, t)$  and  $j(x, t)$  are related to the wave function  $\Psi(x, t)$  by the ordinary definitions  $\rho(x, t) = |\Psi(x, t)|^2$  and  $j(x, t) = \Re[\Psi^*(x, t) (\hbar/i\mu) \Psi(x, t)]$ . When the flux density  $j(x, t)$  changes its sign, quantity  $W(x, t) dt$  is no longer positive-definite and, as in Refs.(Olkhovsky, 1984; Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007), it acquires the physical meaning of a probability density *only* during those partial time-intervals in which the flux

<sup>2</sup> The Naimark theorem states in particular the following(Naimark, 1940): The non-orthogonal spectral decomposition of a maximal hermitian operator can be approximated by an orthogonal spectral function (which corresponds to a selfadjoint operator), in a weak convergence, with any desired accuracy.

<sup>3</sup> Such a condition is enough for operator (1a,b) to be a *hermitian*, or more precisely a *maximal hermitian*[2–8] *operator* (see also (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007)); but it can be dispensed with by recourse to bilinear forms (see, e.g., Refs.(Recami, 1976; 1977; Recami et al., 1983) and refs. therein), as we shall see below.

density  $j(x, t)$  does keep its sign. Therefore, let us introduce the *two* measures (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; 2004; Olkhovsky & Recami, 2007) by separating the positive and the negative flux-direction values (that is, the flux signs)

$$W_{\pm}(t, x) dt = \frac{j_{\pm}(x, t) dt}{\int_{-\infty}^{+\infty} j_{\pm}(x, t) dt} \quad (3)$$

with  $j_{\pm}(x, t) = j(x, t)\theta(\pm j)$ .

Then, the mean value  $\langle t_{\pm}(x) \rangle$  of the time  $t$  at which the particle passes through position  $x$ , when traveling in the positive or negative direction, is, respectively,

$$\langle t_{\pm}(x) \rangle = \frac{\int_{-\infty}^{+\infty} t j_{\pm}(x, t) dt}{\int_{-\infty}^{+\infty} j_{\pm}(x, t) dt} = \frac{\int_0^{+\infty} \frac{1}{2} [G^*(x, E) \hat{t} v G(x, E) + v G^*(x, E) \hat{t} G(x, E)] dE}{\int_0^{+\infty} v |G(x, E)|^2 dE}, \quad (4)$$

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

$$\begin{aligned} \Psi(x, t) &= \int_0^{+\infty} G(x, E) \exp(-iEt/\hbar) dE = \\ &= \int_0^{+\infty} g(E) \varphi(x, E) \exp(-iEt/\hbar) dE \end{aligned}$$

when going on from the time to the energy representation. For free motion, one has  $G(x, E) = g(E) \exp(ikx)$ , and  $\varphi(x, E) = \exp(ikx)$ , while  $E = \mu \hbar^2 k^2 / 2 = \mu v^2 / 2$ . In Refs. (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; 2004; Olkhovsky & Recami, 2007), there were defined the mean time *durations* for the particle 1D transmission from  $x_i$  to  $x_f > x_i$ , and reflection from the region  $(x_i, +\infty)$  back to the interval  $x_f \leq x_i$ . Namely

$$\langle \tau_T(x_i, x_f) \rangle = \langle t_+(x_f) \rangle - \langle t_+(x_i) \rangle \quad (5)$$

and

$$\langle \tau_R(x_i, x_f) \rangle = \langle t_-(x_f) \rangle - \langle t_+(x_i) \rangle, \quad (6)$$

respectively. The 3D generalization for the mean durations of quantum collisions and nuclear reactions appeared in (Olkhovsky, 1984; 1990; 1992; 1998). Finally, suitable definitions of the averages  $\langle t^n \rangle$  on time of  $t^n$ , with  $n = 1, 2, \dots$ , and of  $\langle f(t) \rangle$ , quantity  $f(t)$  being any analytical function of time, can be found in (Olkhovsky & Recami, 2007; 2008), where single-valued expressions have been explicitly written down.

The two canonically conjugate operators, the time operator (1) and the energy operator

$$\hat{E} = \begin{cases} E, & \text{in the energy (E-) representation, (a)} \\ i\hbar \frac{\partial}{\partial t}, & \text{in the time (t-) representation (b)} \end{cases} \quad (7)$$

do clearly satisfy the commutation relation (Olkhovsky & Recami, 2007; 2008; Recami, 1976; 1977)

$$[\hat{E}, \hat{t}] = i\hbar. \quad (8)$$

The Stone and von Neumann theorem (Stone, 1930), has been always interpreted as establishing a commutation relation like (8) for the pair of the canonically conjugate operators (1) and (7), in both representations, for selfadjoint operators only. However, it can be generalized for (maximal) hermitian operators, once one introduces  $\hat{t}$  by means of the *single-valued* Fourier transformation from the  $t$ -axis ( $-\infty < t < \infty$ ) to the  $E$ -semiaxis ( $0 < E < \infty$ ), and utilizes the properties (Akhiezer & Glazman, 1981; D ter Haar, 1971) of the “(maximal) hermitian” operators: This has been shown, e.g., in the last one of Refs. (Olkhovsky & Recami, 1968; 1969) as well as in Refs. (Olkhovsky & Recami, 2007; 2008).

Indeed, from eq. (8) the uncertainty relation

$$\Delta E \Delta t \geq \hbar/2 \quad (9)$$

(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 the average over  $t$  with the measures  $W(x, t) dt$  or  $W_{\pm}(x, t) dt$  in the  $t$ -representation) can be derived also for operators which are simply hermitian, by a straightforward generalization of the procedures which are common in the case of *selfadjoint* (canonically conjugate) quantities, like coordinate  $\hat{x}$  and momentum  $\hat{p}_x$ . Moreover, relation (8) satisfies (Olkhovsky & Recami, 2007; 2008) the Dirac “correspondence” principle, since the classical Poisson brackets  $\{q_0, p_0\}$ , with  $q_0 = t$  and  $p_0 = -E$ , are equal to 1. In Refs. (Olkhovsky, 1973; Olkhovsky et al., 1974; Olkhovsky, 1984; Recami, 1976; 1977), and (Olkhovsky & Recami, 2007; 2008), 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.

As a consequence, one can state that, for systems with continuous energy spectra, the mathematical properties of (maximal) hermitian operators, like  $\hat{t}$  in eq. (1), are sufficient for considering them as quantum observables. Namely, the *uniqueness* (Akhiezer & Glazman, 1981) of the spectral decomposition (although not orthogonal) for operators  $\hat{t}$ , and  $\hat{t}^n$  ( $n > 1$ ), guarantees the “equivalence” of the mean values of any analytical function of time when evaluated in the  $t$  and in the  $E$ -representations. In other words, such an expansion is equivalent to a completeness relation, for the (approximate) eigenfunctions of  $\hat{t}^n$  ( $n > 1$ ), which *with any accuracy* can be regarded as orthogonal, and corresponds to the actual eigenvalues for the continuous spectrum. These approximate eigenfunctions belong to the space of the square-integrable functions of the energy  $E$  (cf., for instance, see, for instance Refs. (Olkhovsky, 1984; 1990; 1992; 1998; Olkhovsky & Recami, 2007; Recami, 1976; 1977) and refs. therein).

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

It is remarkable that von Neumann himself (Von Neumann, 1955), before confining himself for simplicity to selfadjoint operators, stressed that operators like our time  $\hat{t}$  may represent physical observables, even if they are not selfadjoint. Namely, he explicitly considered the example of the operator  $-i\hbar \partial/\partial x$  associated with a particle living in the right semi-space bounded by a rigid wall located at  $x = 0$ ; that operator is not selfadjoint (acting on wave packets defined

on the positive  $x$ -axis) only, nevertheless it obviously corresponds to the  $x$ -component of the observable *momentum* for that particle: See Fig.1.

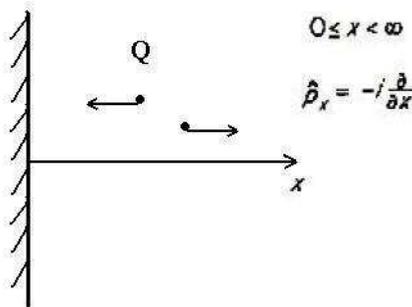


Fig. 1. For a particle  $Q$  free to move in a semi-space, bounded by a rigid wall located at  $x = 0$ , the operator  $-i\partial/\partial x$  has the clear physical meaning of the particle momentum  $x$ -component even if it is *not* selfadjoint (cf. von Neumann (Von Neumann, 1955), and Ref. (Recami, 1976; 1977)): See the text.

At this point, let us emphasize that our previously assumed boundary condition  $E \neq 0$  can be dispensed with, by having recourse (Olkhovsky & Recami, 1968; 1969; Recami, 1976; 1977) to the *bi-linear* hermitian operator

$$\hat{t} = \frac{-i\hbar}{2} \frac{\leftrightarrow}{\partial E} \quad (10)$$

where the meaning of the sign  $\leftrightarrow$  is clear from the accompanying definition

$$(f, \hat{t} g) = \left( f, -\frac{i\hbar}{2} \frac{\partial}{\partial E} g \right) + \left( -\frac{i\hbar}{2} \frac{\partial}{\partial E} f, g \right).$$

By adopting this expression for the time operator, the algebraic sum of the two terms in the r.h.s. of the last relation results to be automatically zero at point  $E = 0$ . This question will be exploited below, in Sect. 3 (when dealing with the more general case of the four-position operator). Incidentally, such an “elimination” (Olkhovsky & Recami, 1968; 1969; Recami, 1976; 1977) of point  $E = 0$  is not only simpler, but also more physical, than other kinds of elimination obtained much later in papers like (Egusquiza & Muga, 1999; Muga et al., 1999).

In connection with the last quotation, let us for briefly comment on the so-called *positive-operator-value-measure* (POVM) approach, often used or discussed in the second set of papers on time in quantum physics mentioned in our Introduction. Actually, an analogous procedure had been proposed, since the sixties (Aharonov & Bohm, 1961), in some approaches to the quantum theory of measurements. Afterwards, and much later, the POVM approach has been applied, in a simplified and shortened form, to the time-operator problem in the case of one-dimensional free motion: for instance, in Refs. (Delgado, 1999; Egusquiza & Muga, 1999; Giannitrapani, 1997; Gózdź A & Dębicki, 2007; Kijowski, 1997; Kobe et al., 1994; Kochański & Wołkievicz, 1999; Leoń, 1997; Muga et al., 1999; Srinivas & Vijayalakshmi, 1981; Toller, 1999; Wang & Xiong, 2007) and especially in (Egusquiza & Muga, 1999; Muga et al., 1999). These papers stated that a generalized decomposition of unity (or “POV measure”) could be obtained from selfadjoint extensions of the time operator inside an extended Hilbert

space (for instance, adding the negative values of the energy, too), by exploiting the Naimark dilation-theorem(Naimark, 1943): But such a program has been realized till now only in the simple cases of one-dimensional particle free motion.

By contrast, our approach is based on a different Naimark's theorem(Naimark, 1940), which, as already mentioned above, allows a much more direct, simple and general –and at the same time non less rigorous– introduction of a quantum operator for Time. More precisely, our approach is based on the so-called *Carleman theorem*(Carleman, 1923), utilized in Ref.(Naimark, 1940), about approximating a hermitian operator by suitable successions of “bounded” selfadjoint operators: That is, of selfadjoint operators whose spectral functions do weakly converge to the non-orthogonal spectral function of the considered hermitian operator. And our approach is applicable to a large family of three-dimensional (3D) particle collisions, with all possible Hamiltonians. Actually, our approach was proposed in the early Refs. (Olkhovsky & Recami, 1968; 1969; 1970; Olkhovsky, 1973; Olkhovsky et al., 1974; Olkhovsky, 1984; Recami, 1976; 1977) and in the first one of Ref. (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995), and applied therein for the time analysis of quantum collisions, nuclear reactions and tunnelling processes.

## 2.2 On the momentum representation of the Time operator

In the continuous spectrum case, instead of the  $E$ -representation, with  $0 < E < +\infty$ , in eqs.(1)–(4) one can also use the  $k$ -representation(Holevo, 1978; 1982), with the advantage that  $-\infty < k < +\infty$ :

$$\Psi(x, t) = \int_{-\infty}^{+\infty} g(k) \varphi(x, k) \exp(-iEt/\hbar) dk \quad (11)$$

with  $E = \hbar^2 k^2 / 2\mu$ , and  $k \neq 0$ .

For the extension of the momentum representation to the case of  $\langle t^n \rangle$ , with  $n > 1$ , we confine ourselves here to refer the reader to the papers (Olkhovsky & Recami, 2007; 2008).

## 2.3 An alternative weight for time averages (in the cases of particle dwelling inside a certain spatial region)

We recall that the weight (2) [as well as its modifications (3)] has the meaning of a probability for the considered particle to pass through point  $x$  during the time interval  $(t, t + dt)$ . Let us follow the procedure presented in Refs. (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007) and refs. therein, and analyze the consequences of the equality

$$\int_{-\infty}^{+\infty} j(x, t) dt = \int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx \quad (12)$$

obtained from the 1D continuity equation. One can easily realize that a second, alternative weight can be adopted:

$$dP(x, t) \equiv Z(x, t) dx = \frac{|\Psi(x, t)|^2 dx}{\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx} \quad (13)$$

which possesses the meaning of probability for the particle to be located (or to sojourn, i. e., to *dwell*) inside the infinitesimal space region  $(x, x + dx)$  at the instant  $t$ , independently of its motion properties. Then, the quantity

$$P(x_1, x_2, t) = \frac{\int_{x_1}^{x_2} |\Psi(x, t)|^2 dx}{\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx} \tag{14}$$

will have the meaning of probability for the particle to dwell inside the spatial interval  $(x_1, x_2)$  at the instant  $t$ .

As it is known (see, for instance, Refs.(Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; 2004; Olkhovsky & Recami, 2007) and refs. therein), the *mean dwell time* can be written in the *two* equivalent forms:

$$\langle \tau(x_i, x_f) \rangle = \frac{\int_{-\infty}^{+\infty} dt \int_{x_i}^{x_f} |\Psi(x, t)|^2 dx}{\int_{-\infty}^{+\infty} j_{in}(x_i, t) dt} \tag{15}$$

and

$$\langle \tau(x_i, x_f) \rangle = \frac{\int_{-\infty}^{+\infty} t j(x_f, t) dt - \int_{-\infty}^{+\infty} t j(x_i, t) dt}{\int_{-\infty}^{+\infty} j_{in}(x_i, t) dt} , \tag{16}$$

where it has been taken account, in particular, of relation (12), which follows — as already said — from the continuity equation.

Thus, in correspondence with the two measures (2) and (13), when integrating over time one gets *two* different kinds of time distributions (mean values, variances...), which refer to the particle traversal time in the case of measure (2), and to the particle dwelling in the case of measure (13). Some examples for 1D tunneling are contained in Refs.(Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; 2004; Olkhovsky & Recami, 2007).

**2.4 Extension of the notion of Time as a quantum-theoretical observable for the case of photons**

As is known (see, for instance, Refs. (Akhiezer & Berestetzky, 1959; Olkhovsky et al., 2004; Schweber, 1961)), in first quantization the single-photon wave function can be probabilistically described in the 1D case by the wave-packet<sup>4</sup>

$$A(\mathbf{r}, t) = \int_{k_0} \frac{d^3k}{k_0} \chi(\mathbf{k}) \varphi(\mathbf{k}, \mathbf{r}) \exp(-ik_0t) , \tag{17}$$

<sup>4</sup> The gauge condition  $\text{div}A = 0$  is assumed.

where, as usual,  $A(\mathbf{r}, t)$  is the electromagnetic vector potential, while  $\mathbf{r} = \{x, y, z\}$ ,  $\mathbf{k} = \{k_x, k_y, k_z\}$ ,  $k_0 \equiv \omega/c = \varepsilon/\hbar c$ , and  $k \equiv |\mathbf{k}| = k_0$ . The axis  $x$  has been chosen as the propagation direction. Let us notice that  $\chi(\mathbf{k}) = \sum_{i=y,z} \chi_i(\mathbf{k}) e_i(\mathbf{k})$ , with  $e_i e_j = \delta_{ij}$ , and  $x_i, x_j = y, z$ , while  $\chi_i(\mathbf{k})$  is the probability amplitude for the photon to have momentum  $\mathbf{k}$  and polarization  $e_j$  along  $x_j$ . Moreover, it is  $\varphi(\mathbf{k}, \mathbf{r}) = \exp(ik_x x)$  in the case of plane waves, while  $\varphi(\mathbf{k}, \mathbf{r})$  is a linear combination of evanescent (decreasing) and anti-evanescent (increasing) waves in the case of "photon barriers" (i.e., band-gap filters, or even undersized segments of waveguides for microwaves, or frustrated total-internal-reflection regions for light, and so on). Although it is not easy to localize a photon in the direction of its polarization (Akhiezer & Berestezky, 1959; Schweber, 1961), nevertheless for 1D propagations it is possible to use the space-time probabilistic interpretation of eq. (17), and define the quantity

$$\rho_{em}(x, t) dx = \frac{S_0 dx}{\int S_0 dx}, \quad S_0 = \iint s_0 dy dz \quad (18)$$

( $s_0 = [\mathbf{E}^* \cdot \mathbf{E} + \mathbf{H}^* \cdot \mathbf{H}]/4\pi$  being the energy density, with the electromagnetic field  $\mathbf{H} = \text{rot } \mathbf{A}$ , and  $\mathbf{E} = -1/c \partial \mathbf{A}/\partial t$ ), which represents the probability density of a photon to be found (localized) in the spatial interval  $(x, x + dx)$  along the  $x$ -axis at the instant  $t$ ; and the quantity

$$j_{em}(x, t) dt = \frac{S_x dt}{\int S_x(x, t) dt}, \quad S_x(x, t) = \iint s_x dy dz \quad (19)$$

( $s_x = c \Re[\mathbf{E}^* \wedge \mathbf{H}]_x / 8\pi$  being the energy flux density), which represents the flux probability density of a photon to pass through point  $x$  in the time interval  $(t, t + dt)$ : in full analogy with the probabilistic quantities for non-relativistic particles. The justification and convenience of such definitions is self-evident, when the wave-packet group velocity coincides with the velocity of the energy transport; in particular: (i) the wave-packet (17) is quite similar to wave-packets for non-relativistic particles, and (ii) in analogy with conventional non-relativistic quantum mechanics, one can define the "mean time instant" for a photon (i.e., an electromagnetic wave-packet) to pass through point  $x$ , as follows

$$\langle t(x) \rangle = \int_{-\infty}^{+\infty} t J_{em,x} dt = \frac{\int_{-\infty}^{+\infty} t S_x(x, t) dt}{\int_{-\infty}^{+\infty} S_x(x, t) dt}.$$

As a consequence [in the same way as in the case of equations (1)–(2)], the form (1) for the time operator in the energy representation is valid also for photons, with the same boundary conditions adopted in the case of particles, that is, with  $\chi_i(0) = \chi_i(\infty)$  and with  $E = \hbar c k_0$ . The energy density  $s_0$  and energy flux density  $s_x$  satisfy the relevant continuity equation

$$\frac{\partial s_0}{\partial t} + \frac{\partial s_x}{\partial x} = 0 \quad (20)$$

which is Lorentz-invariant for 1D spatial propagation (Olkhovsky et al., 2004; Olkhovskiy & Recami, 2007) processes.

### 2.5 Introducing the analogue of the “Hamiltonian” for the case of the Time operator: A new hamiltonian approach

In non-relativistic quantum theory, the Energy operator acquires (cf., e.g., Refs. (Olkhovsky, 1990; 1992; 1998; Olkhovskiy & Recami, 2007)) the *two* forms: (i)  $i\hbar \frac{\partial}{\partial t}$  in the  $t$ -representation, and (ii)  $\hat{H}(\hat{p}_x, \hat{x}, \dots)$  in the hamiltonian formalism. The “duality” of these two forms can be easily inferred from the Schrödinger equation itself,  $\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$ . One can introduce in quantum mechanics a similar duality for the case of *Time*: Besides the general form (1) for the Time operator in the energy representation, which is valid for any physical systems in the region of continuous energy spectra, one can express the time operator also in a “hamiltonian form”, i.e., in terms of the coordinate and momentum operators, by having recourse to their commutation relations. Thus, by the replacements

$$\begin{aligned}\hat{E} &\rightarrow \hat{H}(\hat{p}_x, \hat{x}, \dots), \\ \hat{t} &\rightarrow \hat{T}(\hat{p}_x, \hat{x}, \dots),\end{aligned}\tag{21}$$

and on using the commutation relation [similar to eq. (3)]

$$[\hat{H}, \hat{T}] = i\hbar,\tag{22}$$

one can obtain (Rosenbaum, 1969), given a specific ordinary Hamiltonian, the corresponding explicit expression for  $\hat{T}(\hat{p}_x, \hat{x}, \dots)$ .

Indeed, this procedure can be adopted for any physical system with a known Hamiltonian  $\hat{H}(\hat{p}_x, \hat{x}, \dots)$ , and we are going to see a concrete example. By going on from the coordinate to the momentum representation, one realizes that the *formal* expressions of *both* the hamiltonian-type operators  $\hat{H}(\hat{p}_x, \hat{x}, \dots)$  and  $\hat{T}(\hat{p}_x, \hat{x}, \dots)$  do not change, except for an obvious change of sign in the case of operator  $\hat{T}(\hat{p}_x, \hat{x}, \dots)$ .

As an explicit example, let us address the simple case of a free particle whose Hamiltonian is

$$\hat{H} = \begin{cases} \hat{p}_x^2 / 2\mu, & \hat{p}_x = -i\hbar \frac{\partial}{\partial x}, & \text{in the coordinate representation (a)} \\ p_x^2 / 2\mu. & & \text{in the momentum representation (a)} \end{cases}\tag{23}$$

Correspondingly, the Hamilton-type *time operator*, in its symmetrized form, will write

$$\hat{T} = \begin{cases} \frac{\mu}{2} (\hat{p}_x^{-1} x + x \hat{p}_x^{-1} + i\hbar; \hat{p}_x^{-2}), & \text{in the coordinate representation (a)} \\ -\frac{\mu}{2} (p_x^{-1} \hat{x} + \hat{x} p_x^{-1} + i\hbar / p_x^2), & \text{in the momentum representation (b)} \end{cases}\tag{24}$$

where

$$\hat{p}_x^{-1} = \frac{i}{\hbar} \int dx \dots, \quad \hat{x} = i\hbar \frac{\partial}{\partial p_x}.$$

Incidentally, operator (24b) is equivalent to  $-i\hbar \frac{\partial}{\partial E}$ , since  $E = p_x^2 / 2\mu$ ; and therefore it is also a (maximal) *hermitian* operator. Indeed, by applying the operator  $\hat{T}(\hat{p}_x, \hat{x}, \dots)$ , for instance, to a plane-wave of the type  $\exp(ikx)$ , we obtain the same result in both the coordinate and the momentum representations:

$$\hat{T} \exp(ikx) = \frac{x}{v} \exp(ikx)\tag{25}$$

quantity  $x/v$  being the free-motion time (for a particle with velocity  $v$ ) for traveling the distance  $x$ .

On the basis of what precedes, it is possible to show that the wave function  $\Psi(x, t)$  of a quantum system satisfies the two (dual) equations

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \text{ and } \hat{T}\Psi = t\Psi. \quad (26)$$

In the energy representation, and in the stationary case, we obtain again *two* (dual) equations

$$\hat{H}\varphi_\varepsilon = \varepsilon\varphi_\varepsilon \text{ and } \hat{T}\varphi_\varepsilon = -i\hbar \frac{\partial \varphi_\varepsilon}{\partial \varepsilon}, \quad (27)$$

quantity  $\varphi_\varepsilon$  being the Fourier-transform of  $\Psi$ :

$$\varphi_\varepsilon = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} \Psi(x, t) e^{i\varepsilon t/\hbar} dt. \quad (28)$$

It might be interesting to apply the two pairs of the last dual equations also for investigating tunnelling processes through the quantum gravitational barrier, which appears during inflation, or at the beginning of the big-bang expansion, whenever a quasi-linear Schrödinger-type equation does approximately show up.

## 2.6 Time as an observable (and the time-energy uncertainty relation), for quantum-mechanical systems with discrete energy spectra

For describing the time evolution of non-relativistic quantum systems endowed with a purely *discrete* (or a continuous *and discrete*) spectrum, let us now introduce wave-packets of the form (Olkhovsky, 1990; 1992; 1998; Olkhovsky & Recami, 2007; 2008):

$$\psi(x, t) = \sum_{n=0} g_n \varphi_n(x) \exp[-i(\varepsilon_n - \varepsilon_0)t/\hbar], \quad (29)$$

where  $\varphi_n(x)$  are orthogonal and normalized bound states which satisfy the equation  $\hat{H}\varphi_n(x) = \varepsilon_n \varphi_n(x)$ , quantity  $\hat{H}$  being the Hamiltonian of the system; while the coefficients  $g_n$  are normalized:  $\sum_{n=0} |g_n|^2 = 1$ . We omitted the non-significant phase factor  $\exp(-i\varepsilon_0 t/\hbar)$  of the fundamental state.

Let us first consider the systems whose energy levels are separated by intervals admitting a maximum common divisor  $D$  (for ex., harmonic oscillator, particle in a rigid box, and spherical spinning top), so that the wave packet (29) is a periodic function of time possessing as period the Poincaré cycle time  $T = 2\pi\hbar/D$ . For such systems it is possible (Olkhovsky, 1990; 1992; 1998; Olkhovsky & Recami, 2007; 2008) to construct a *selfadjoint* time operator with the form (in the time representation) of a saw-function of  $t$ , choosing  $t = 0$  as the initial time instant:

$$\hat{t} = t - T \sum_{n=0}^{\infty} \Theta(t - [2n + 1]T/2) + T \sum_{n=0}^{\infty} \Theta(-t - [2n + 1]T/2). \quad (30)$$

This periodic function for the time operator is a linear (increasing) function of time  $t$  within each Poincaré cycle: see Fig.2.

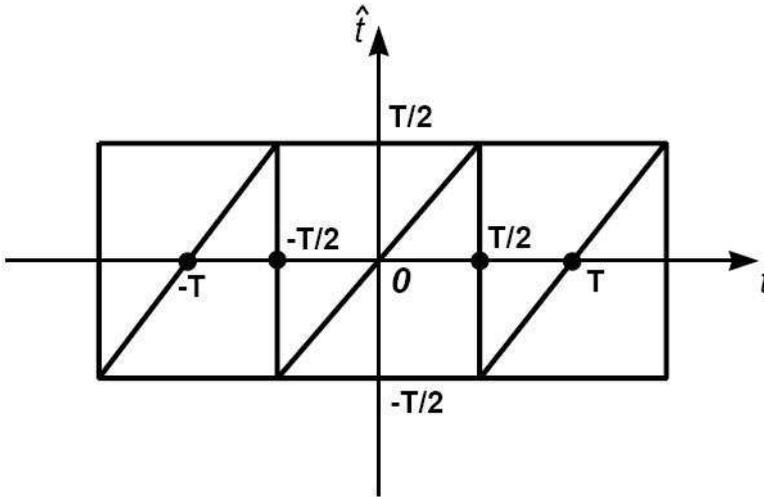


Fig. 2. The periodic saw-tooth function for the time operator in the case of quantum mechanical systems with *discrete* energy spectra: Namely, for the case of eq. (30).

The commutation relations of the Energy and Time operators, now both selfjoint, acquires in the case of discrete energies and of a periodic Time operator the form

$$[\hat{E}, \hat{t}] = i\hbar \left\{ 1 - T \sum_{n=0}^{\infty} \delta(t - [2n + 1]T) \right\}, \tag{31}$$

wherefrom the uncertainty relation follows in the new form

$$(\Delta E)^2 (\Delta t)^2 = \hbar^2 \left[ 1 - \frac{T |\psi(T/2 + \gamma)|^2}{\int_{-T/2}^{T/2} |\psi(t)|^2 dt} \right], \tag{32}$$

where it has been introduced a parameter  $\gamma$ , with  $-T/2 < \gamma < T/2$ , in order to assure that the r.h.s. integral is single-valued(Olkhovsky & Recami, 2007; 2008).

When  $\Delta E \rightarrow 0$  (that is, when  $|g_n| \rightarrow \delta_{nm}$ ), the r.h.s. of eq. (32) tends to zero too, since  $|\psi(t)|^2$  tends to a constant value. In such a case, the distribution of the time instants at which the wave-packet passes through point  $x$  becomes flat within each Poincaré cycle. When, by contrast,  $\Delta E \gg D$  and  $|\psi(T + \gamma)|^2 \ll (\int_{-T/2}^{T/2} |\psi(t)|^2 dt)/T$ , the periodicity condition may become inessential whenever  $\Delta t \ll t$ . In other words, our uncertainty relation (32) transforms into the ordinary uncertainty relation for systems with continuous spectra.

In more general cases, for excited states of nuclei, atoms and molecules, the *energy-level intervals, for discrete and quasi-discrete (resonance) spectra, are not multiples of a maximum common divisor*, and hence the Poincaré cycle is not well-defined for such systems. Nevertheless, even for those systems one can introduce an approximate description (sometimes, with any desired degree of accuracy) in terms of Poincaré quasi-cycles and a quasi-periodical evolution; so that for sufficiently long time intervals the behavior of the wave-packets can be associated with a *periodical motion (oscillation)*, sometimes — e.g., for very narrow resonances — with any desired

accuracy. For them, when choosing an approximate Poincaré-cycle time, one can include in one cycle as many quasi-cycles as it is necessary for the demanded accuracy. Then, with the chosen accuracy, a *quasi-selfadjoint time operator* can be introduced.

### 3. Multiple internal reflections approach in description of tunneling

#### 3.1 Tunneling in consideration of multiple internal reflections of waves between internal boundaries

An approach for description of one-dimensional motion of a non-relativistic particle above a barrier on the basis of multiple internal reflections of stationary waves relatively boundaries has been studied in number of papers and is known (see (Anderson, 1989; Fermor, 1966; McVoy et al., 1967) and references therein). Tunneling of the particle under the barrier was described successfully on the basis of multiple internal reflections of the wave packets relatively boundaries (approach was called as *method of multiple internal reflections* or *method MIR*, see Refs. (Maydanyuk et al., 2002a;b; Maydanyuk, 2003; Olkhovsky, 2000)). In such approach it succeeded in connecting: 1) continuous transition of solutions for packets after each reflection, total packets between the above-barrier motion and the under-barrier tunneling; 2) coincidence of transmitted and reflected amplitudes of stationary wave function in each spatial region obtained by approach MIR with the corresponding amplitudes obtained by standard method of quantum mechanics; 3) all non-stationary fluxes in each step, are non-zero that confirms propagation of packets under the barrier (i. e. their “tunneling”). In frameworks of such a method, non-stationary tunneling obtained own interpretation, allowing to study this process at interesting time moment or space point. In calculation of phase times this method turns out to be enough simple and convenient (Cardone et al., 2006). It has been adapted for scattering of the particle on nucleus and  $\alpha$ -decay in the spherically symmetric approximation with the simplest radial barriers (Maydanyuk et al., 2002a; Maydanyuk, 2003; Olkhovsky, 2000) and for tunneling of photons (Cardone et al., 2006; Maydanyuk et al., 2002a). However, further realization of the MIR approach meets with three questions. 1) *Question on effectiveness*. The multiple reflections have been proved for the motion above one rectangular barrier and for tunneling under it (Anderson, 1989; Cardone et al., 2006; Maydanyuk et al., 2002a). However, after addition of the second step it becomes unclear how to separate the needed reflected waves from all their variety in calculation of all needed amplitudes. After obtaining exact solutions of the stationary amplitudes for two arbitrary rectangular barriers (Maydanyuk, 2003; Olkhovsky, 2000), it becomes unclear how to generalize such approach for barriers with arbitrary complicate shape. So, *we come to a serious unresolved problem of realization of the approach of multiple reflections in real quantum systems with complicated barriers*, and clear algorithms of calculation of amplitudes should be constructed. 2) *Question on correctness*. Whether is interference between packets formed relatively different boundaries appeared? Whether does this come to principally different results of the approach of multiple internal reflections and direct methods of quantum mechanics? Note that such interference cannot be appeared in tunneling through one rectangular barrier and, therefore, it could not visible in the previous papers. 3) *Question on uncertainty in radial problem*. Calculations of half-lives of different types of decays based on the semiclassical approach are prevailing today. For example, in Ref. (Buck et al., 1993) agreement between experimental data of  $\alpha$ -decay half-lives and ones calculated by theory is demonstrated in a wide region of nuclei from  $^{106}\text{Te}$  up to nucleus with  $A_d = 266$  and  $Z_d = 109$  (see Ref. (Denisov & Ikezoe, 2005) for some improved approaches). In review (Sobiczewski & Pomorski, 2007) methodology of calculation of half-lives for

spontaneous-fission is presented (see eqs. (21)–(24) in p. 321). Let us consider proton-decay of nucleus where proton penetrates from the internal region outside with its tunneling through the barrier. At the same boundary condition, reflected and incident waves turn out to be defined with uncertainty. How to determine them? The semiclassical approach gives such answer: *according to theory, in construction of well known formula for probability we neglect completely by the second (increasing) item of the wave function inside tunneling region* (see Ref. (Landau & Lifshitz, 1989), eq. (50.2), p. 221). In result, equality  $T^2 + R^2 = 1$  has no any sense (where  $T$  and  $R$  are coefficients of penetrability and reflection). Condition of continuity for the wave function and for total flux is broken at turning point. So, we do not find reflection  $R$ . We do not suppose on possible interference between incident and reflected waves which can be non zero. The penetrability is determined by the barrier shape inside tunneling region, while internal and external parts do not take influence on it. The penetrability does not dependent on depth of the internal well (while the simplest rectangular well and barrier give another exact result). But, the semiclassical approach is so prevailing that one can suppose that it has enough well approximation of the penetrability estimated. It turns out that if in fully quantum approach to determine the penetrability through the barrier (constructed on the basis of realistic potential of interaction between proton and daughter nucleus) then one can obtain answer “no”. Fully quantum penetrability is a function of new additional independent parameters, it can achieve essential difference from semiclassical one (at the same boundary condition imposed on the wave function). This will be demonstrated below.

### 3.2 Tunneling of packet through one-dimensional rectangular step

Let us consider a problem of tunneling of a particle in a positive  $x$ -direction through an one-dimensional rectangular potential barrier (see Fig. 3). Let us label a region I for  $x < 0$ , a region II for  $0 < x < a$  and a region III for  $x > a$ , accordingly. In standard approach, with

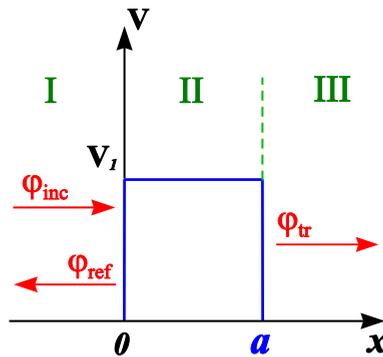


Fig. 3. Tunneling of the particle through one-dimensional rectangular barrier

energy less than the barrier height the tunneling evolution of the particle is described using a non-stationary propagation of WP

$$\psi(x, t) = \int_0^{+\infty} g(E - \bar{E}) \varphi(k, x) e^{-iEt/\hbar} dE, \quad (33)$$

where stationary WF is:

$$\varphi(x) = \begin{cases} e^{ikx} + A_R e^{-ikx}, & \text{for } x < 0; \\ \alpha e^{\xi x} + \beta e^{-\xi x}, & \text{for } 0 < x < a; \\ A_T e^{ikx}, & \text{for } x > a; \end{cases} \quad (34)$$

and  $k = \frac{1}{\hbar} \sqrt{2mE}$ ,  $\xi = \frac{1}{\hbar} \sqrt{2m(V_1 - E)}$ ,  $E$  and  $m$  are the total energy and mass of the particle, accordingly. The weight amplitude  $g(E - \bar{E})$  can be written in a form of gaussian and satisfies to a requirement of the normalization  $\int |g(E - \bar{E})|^2 dE = 1$ , value  $\bar{E}$  is an average energy of the particle. One can calculate coefficients  $A_T$ ,  $A_R$ ,  $\alpha$  and  $\beta$  analytically, using a requirements of a continuity of WF  $\varphi(x)$  and its derivative on each boundary of the barrier. Substituting in eq. (33) instead of  $\varphi(k, x)$  the incident  $\varphi_{inc}(k, x)$ , transmitted  $\varphi_{tr}(k, x)$  or reflected part of WF  $\varphi_{ref}(k, x)$ , defined by eq. (34), we receive the incident, transmitted or reflected WP, accordingly.

We assume, that a time, for which the WP tunnels through the barrier, is enough small. So, the time necessary for a tunneling of proton through a barrier of decay in proton-decay of a nucleus, is about  $10^{-21}$  seconds. We consider, that one can neglect a spreading of the WP for this time. And a breadth of the WP appears essentially more narrow on a comparison with a barrier breadth. Considering only sub-barrier processes, we exclude a component of waves for above-barrier energies, having included the additional transformation

$$g(E - \bar{E}) \rightarrow g(E - \bar{E})\theta(V_1 - E), \quad (35)$$

where  $\theta$ -function satisfies to the requirement

$$\theta(\eta) = \begin{cases} 0, & \text{for } \eta < 0; \\ 1, & \text{for } \eta > 0. \end{cases}$$

The method of multiple internal reflections considers the propagation process of the WP describing a motion of the particle, sequentially on steps of its penetration in relation to each boundary of the barrier (Anderson, 1989; Fermor, 1966; McVoy et al., 1967). Using this method, we find expressions for the transmitted and reflected WP in relation to the barrier. At the first step we consider the WP in the region I, which is incident upon the first (initial) boundary of the barrier. Let us assume, that this package transforms into the WP, transmitted through this boundary and tunneling further in the region II, and into the WP, reflected from the boundary and propagating back in the region I. Thus we consider, that the WP, tunneling in the region II, is not reached the second (final) boundary of the barrier because of a terminating velocity of its propagation, and consequently at this step we consider only two regions I and II. Because of physical reasons to construct an expression for this packet, we consider, that its amplitude should decrease in a positive  $x$ -direction. We use only one item  $\beta \exp(-\xi x)$  in eq. (34), throwing the second increasing item  $\alpha \exp(\xi x)$  (in an opposite case we break a requirement of a finiteness of the WF for an indefinitely wide barrier). In result, in the region II we obtain:

$$\psi_{tr}^1(x, t) = \int_0^{+\infty} g(E - \bar{E})\theta(V_1 - E)\beta^0 e^{-\xi x - iEt/\hbar} dE, \text{ for } 0 < x < a. \quad (36)$$

Thus the WF in the barrier region constructed by such way, is an analytic continuation of a relevant expression for the WF, corresponding to a similar problem with above-barrier

energies, where as a stationary expression we select the wave  $\exp(ik_2x)$ , propagated to the right.

Let us consider the first step further. One can write expressions for the incident and the reflected WP in relation to the first boundary as follows

$$\begin{aligned}\psi_{inc}(x, t) &= \int_0^{+\infty} g(E - \bar{E})\theta(V_1 - E)e^{ikx - iEt/\hbar} dE, & \text{for } x < 0, \\ \psi_{ref}^1(x, t) &= \int_0^{+\infty} g(E - \bar{E})\theta(V_1 - E)A_R^0 e^{-ikx - iEt/\hbar} dE, & \text{for } x < 0.\end{aligned}\quad (37)$$

A sum of these expressions represents the complete WF in the region I, which is dependent on a time. Let us require, that this WF and its derivative continuously transform into the WF (36) and its derivative at point  $x = 0$  (we assume, that the weight amplitude  $g(E - \bar{E})$  differs weakly at transmitting and reflecting of the WP in relation to the barrier boundaries). In result, we obtain two equations, in which one can pass from the time-dependent WP to the corresponding stationary WF and obtain the unknown coefficients  $\beta^0$  and  $A_R^0$ .

At the second step we consider the WP, tunneling in the region II and incident upon the second boundary of the barrier at point  $x = a$ . It transforms into the WP, transmitted through this boundary and propagated in the region III, and into the WP, reflected from the boundary and tunneled back in the region II. For a determination of these packets one can use eq. (33) with account eq. (35), where as the stationary WF we use:

$$\begin{aligned}\varphi_{inc}^2(k, x) &= \varphi_{tr}^1(k, x) = \beta^0 e^{-\xi x}, & \text{for } 0 < x < a, \\ \varphi_{tr}^2(k, x) &= A_T^0 e^{ikx}, & \text{for } x > a, \\ \varphi_{ref}^2(k, x) &= \alpha^0 e^{\xi x}, & \text{for } 0 < x < a.\end{aligned}\quad (38)$$

Here, for forming an expression for the WP reflected from the boundary, we select an increasing part of the stationary solution  $\alpha^0 \exp(\xi x)$  only. Imposing a condition of continuity on the time-dependent WF and its derivative at point  $x = a$ , we obtain 2 new equations, from which we find the unknowns coefficients  $A_T^0$  and  $\alpha^0$ .

At the third step the WP, tunneling in the region II, is incident upon the first boundary of the barrier. Then it transforms into the WP, transmitted through this boundary and propagated further in the region I, and into the WP, reflected from boundary and tunneled back in the region II. For a determination of these packets one can use eq. (33) with account eq. (35), where as the stationary WF we use:

$$\begin{aligned}\varphi_{inc}^3(k, x) &= \varphi_{ref}^2(k, x), & \text{for } 0 < x < a, \\ \varphi_{tr}^3(k, x) &= A_R^1 e^{-ikx}, & \text{for } x < 0, \\ \varphi_{ref}^3(k, x) &= \beta^1 e^{-\xi x}, & \text{for } 0 < x < a.\end{aligned}\quad (39)$$

Using a conditions of continuity for the time-dependent WF and its derivative at point  $x = 0$ , we obtain the unknowns coefficients  $A_R^1$  and  $\beta^1$ .

Analyzing further possible processes of the transmission (and the reflection) of the WP through the boundaries of the barrier, we come to a deduction, that any of following steps can be reduced to one of 2 considered above. For the unknown coefficients  $\alpha^n$ ,  $\beta^n$ ,  $A_T^n$  and  $A_R^n$ , used in expressions for the WP, forming in result of some internal reflections from the

boundaries, one can obtain the recurrence relations:

$$\begin{aligned}\beta^0 &= \frac{2k}{k+i\zeta}, \quad \alpha^n = \beta^n \frac{i\zeta - k}{i\zeta + k} e^{-2\zeta a}, \quad \beta^{n+1} = \alpha^n \frac{i\zeta - k}{i\zeta + k}, \\ A_R^0 &= \frac{k-i\zeta}{k+i\zeta}, \quad A_T^n = \beta^n \frac{2i\zeta}{i\zeta + k} e^{-\zeta a - ika}, \quad A_R^{n+1} = \alpha^n \frac{2i\zeta}{i\zeta + k}.\end{aligned}\quad (40)$$

Considering the propagation of the WP by such way, we obtain expressions for the WF on each region which can be written through series of multiple WP. Using eq. (33) with account eq. (35), we determine resultant expressions for the incident, transmitted and reflected WP in relation to the barrier, where one can need to use following expressions for the stationary WF:

$$\begin{aligned}\varphi_{inc}(k, x) &= e^{ikx}, \quad \text{for } x < 0, \\ \varphi_{tr}(k, x) &= \sum_{n=0}^{+\infty} A_T^n e^{ikx}, \quad \text{for } x > a, \\ \varphi_{ref}(k, x) &= \sum_{n=0}^{+\infty} A_R^n e^{-ikx}, \quad \text{for } x < 0.\end{aligned}\quad (41)$$

Now we consider the WP formed in result of sequential  $n$  reflections from the boundaries of the barrier and incident upon one of these boundaries at point  $x = 0$  ( $i = 1$ ) or at point  $x = a$  ( $i = 2$ ). In result, this WP transforms into the WP  $\psi_{tr}^i(x, t)$ , transmitted through boundary with number  $i$ , and into the WP  $\psi_{ref}^i(x, t)$ , reflected from this boundary. For an independent on  $x$  parts of the stationary WF one can write:

$$\begin{aligned}\frac{\varphi_{tr}^1}{\exp(-\zeta x)} &= T_1^+ \frac{\varphi_{inc}^1}{\exp(ikx)}, \quad \frac{\varphi_{ref}^1}{\exp(-ikx)} = R_1^+ \frac{\varphi_{inc}^1}{\exp(ikx)}, \\ \frac{\varphi_{tr}^2}{\exp(ikx)} &= T_2^+ \frac{\varphi_{inc}^2}{\exp(-\zeta x)}, \quad \frac{\varphi_{ref}^2}{\exp(\zeta x)} = R_2^+ \frac{\varphi_{inc}^2}{\exp(-\zeta x)}, \\ \frac{\varphi_{tr}^1}{\exp(-ikx)} &= T_1^- \frac{\varphi_{inc}^1}{\exp(\zeta x)}, \quad \frac{\varphi_{ref}^1}{\exp(-\zeta x)} = R_1^- \frac{\varphi_{inc}^1}{\exp(\zeta x)},\end{aligned}\quad (42)$$

where the sign “+” (or “-”) corresponds to the WP, tunneling (or propagating) in a positive (or negative)  $x$ -direction and incident upon the boundary with number  $i$ . Using  $T_i^\pm$  and  $R_i^\pm$ , one can precisely describe an arbitrary WP which has formed in result of  $n$ -multiple reflections, if to know a “path” of its propagation along the barrier. Using the recurrence relations eq. (40), the coefficients  $T_i^\pm$  and  $R_i^\pm$  can be obtained.

$$\begin{aligned}T_1^+ &= \beta^0, \quad T_2^+ = \frac{A_T^n}{\beta^n}, \quad T_1^- = \frac{A_R^{n+1}}{\alpha^n}, \\ R_1^+ &= A_R^0, \quad R_2^+ = \frac{\alpha^n}{\beta^n}, \quad R_1^- = \frac{\beta^{n+1}}{\alpha^n}.\end{aligned}\quad (43)$$

Using the recurrence relations, one can find series of coefficients  $\alpha^n, \beta^n, A_T^n$  and  $A_R^n$ . However, these series can be calculated easier, using coefficients  $T_i^\pm$  and  $R_i^\pm$ . Analyzing all possible

“paths” of the WP propagations along the barrier, we receive:

$$\begin{aligned}
 \sum_{n=0}^{+\infty} A_T^n &= T_2^+ T_1^- \left( 1 + \sum_{n=1}^{+\infty} (R_2^+ R_1^-)^n \right) = \frac{i4k\zeta e^{-\zeta a - ika}}{F_{sub}}, \\
 \sum_{n=0}^{+\infty} A_R^n &= R_1^+ + T_1^+ R_2^+ T_1^- \left( 1 + \sum_{n=1}^{+\infty} (R_2^+ R_1^-)^n \right) = \frac{k_0^2 D_-}{F_{sub}}, \\
 \sum_{n=0}^{+\infty} \alpha^n &= \alpha^0 \left( 1 + \sum_{n=1}^{+\infty} (R_2^+ R_1^-)^n \right) = \frac{2k(i\zeta - k)e^{-2\zeta a}}{F_{sub}}, \\
 \sum_{n=0}^{+\infty} \beta^n &= \beta^0 \left( 1 + \sum_{n=1}^{+\infty} (R_2^+ R_1^-)^n \right) = \frac{2k(i\zeta + k)}{F_{sub}},
 \end{aligned}
 \tag{44}$$

where

$$\begin{aligned}
 F_{sub} &= (k^2 - \zeta^2)D_- + 2ik\zeta D_+, \\
 D_{\pm} &= 1 \pm e^{-2\zeta a}, \\
 k_0^2 &= k^2 + \zeta^2 = \frac{2mV_1}{\hbar^2}.
 \end{aligned}
 \tag{45}$$

All series  $\sum \alpha^n$ ,  $\sum \beta^n$ ,  $\sum A_T^n$  and  $\sum A_R^n$ , obtained using the method of multiple internal reflections, coincide with the corresponding coefficients  $\alpha$ ,  $\beta$ ,  $A_T$  and  $A_R$  of the eq. (34), calculated by a stationary methods. Using the following substitution

$$i\zeta \rightarrow k_2, \tag{46}$$

where  $k_2 = \frac{1}{\hbar} \sqrt{2m(E - V_1)}$  is a wave number for a case of above-barrier energies, expression for the coefficients  $\alpha^n$ ,  $\beta^n$ ,  $A_T^n$  and  $A_R^n$  for each step, expressions for the WF for each step, the total eqs. (44) and (45) transform into the corresponding expressions for a problem of the particle propagation above this barrier. At the transformation of the WP and the time-dependent WF one can need to change a sign of argument at  $\theta$ -function. Besides the following property is fulfilled:

$$\left| \sum_{n=0}^{+\infty} A_T^n \right|^2 + \left| \sum_{n=0}^{+\infty} A_R^n \right|^2 = 1. \tag{47}$$

**3.3 Exact solutions for wave function for tunneling through radial barrier composed from arbitrary number of potential steps**

Now we shall come to radial problem (Maydanyuk & Belchikov, 2011). Let us assume that starting from some time moment before decay the nucleus could be considered as system composite from daughter nucleus and fragment emitted. Its decay is described by a particle with reduced mass  $m$  which moves in radial direction inside a radial potential with a barrier. We shall be interesting in the radial barrier of arbitrary shape, which has successfully been approximated by finite number  $N$  of rectangular steps:

$$V(r) = \begin{cases} V_1, & \text{at } R_{\min} < r \leq r_1 & \text{(region 1),} \\ V_2, & \text{at } r_1 \leq r \leq r_2 & \text{(region 2),} \\ \dots & \dots & \dots \\ V_N, & \text{at } r_{N-1} \leq r \leq R_{\max} & \text{(region N),} \end{cases} \tag{48}$$

where  $V_i$  are constants ( $i = 1 \dots N$ ). We define the first region 1 starting from point  $R_{\min}$ , assuming that the fragment is formed here and then it moves outside. We shall be interesting

in solutions for above barrier energies while the solution for tunneling could be obtained after by change  $i \zeta_i \rightarrow k_i$ . A general solution of the wave function (up to its normalization) has the following form:

$$\psi(r, \theta, \varphi) = \frac{\chi(r)}{r} Y_{lm}(\theta, \varphi), \quad (49)$$

$$\chi(r) = \begin{cases} e^{ik_1 r} + A_R e^{-ik_1 r}, & \text{at } R_{\min} < r \leq r_1 \quad (\text{region 1}), \\ \alpha_2 e^{ik_2 r} + \beta_2 e^{-ik_2 r}, & \text{at } r_1 \leq r \leq r_2 \quad (\text{region 2}), \\ \dots & \dots \quad \dots \\ \alpha_{n-1} e^{ik_{N-1} r} + \beta_{N-1} e^{-ik_{N-1} r}, & \text{at } r_{N-2} \leq r \leq r_{N-1} \quad (\text{region } N-1), \\ A_T e^{ik_N r}, & \text{at } r_{N-1} \leq r \leq R_{\max} \quad (\text{region } N), \end{cases} \quad (50)$$

where  $\alpha_j$  and  $\beta_j$  are unknown amplitudes,  $A_T$  and  $A_R$  are unknown amplitudes of transmission and reflection,  $Y_{lm}(\theta, \varphi)$  is spherical function,  $k_i = \frac{1}{\hbar} \sqrt{2m(E - V_i)}$  are complex wave numbers. We shall be looking for solution for such problem in approach of multiple internal reflections (we restrict ourselves by a case of orbital moment  $l = 0$  while its non-zero generalization changes the barrier shape which was used as arbitrary before in development of formalism MIR and, so, is absolutely non principal).

According to the method of multiple internal reflections, scattering of the particle on the barrier is considered on the basis of wave packet consequently by steps of its propagation relatively to each boundary of the barrier (the most clearly idea of such approach can be understood in the problem of tunneling through the simplest rectangular barrier, see (Cardone et al., 2006; Maydanyuk et al., 2002a; Maydanyuk, 2003) where one can find proof of this fully quantum exactly solvable method, one can analyze its properties). Each step in such consideration of propagation of the packet will be similar to one from the first  $2N - 1$  steps, independent between themselves. From analysis of these steps recurrent relations are found for calculation of unknown amplitudes  $A^{(n)}$ ,  $S^{(n)}$ ,  $\alpha^{(n)}$  and  $\beta^{(n)}$  for arbitrary step  $n$ , summation of these amplitudes are calculated. We shall be looking for the unknown amplitudes, requiring wave function and its derivative to be continuous at each boundary. We shall consider the coefficients  $T_1^\pm, T_2^\pm, T_3^\pm \dots$  and  $R_1^\pm, R_2^\pm, R_3^\pm \dots$  as additional factors to amplitudes  $e^{\pm i k x}$ . Here, bottom index denotes number of the boundary, upper (top) signs “+” and “-” denote directions of the wave to the right or to the left, correspondingly. At the first, we calculate  $T_1^\pm, T_2^\pm \dots T_{N-1}^\pm$  and  $R_1^\pm, R_2^\pm \dots R_{N-1}^\pm$ :

$$\begin{aligned} T_j^+ &= \frac{2k_j}{k_j + k_{j+1}} e^{i(k_j - k_{j+1})r_j}, & T_j^- &= \frac{2k_{j+1}}{k_j + k_{j+1}} e^{i(k_j - k_{j+1})r_j}, \\ R_j^+ &= \frac{k_j - k_{j+1}}{k_j + k_{j+1}} e^{2ik_j r_j}, & R_j^- &= \frac{k_{j+1} - k_j}{k_j + k_{j+1}} e^{-2ik_{j+1} r_j}. \end{aligned} \quad (51)$$

Using recurrent relations:

$$\begin{aligned} \tilde{R}_{j-1}^+ &= R_{j-1}^+ + T_{j-1}^+ \tilde{R}_j^+ T_{j-1}^- \left( 1 + \sum_{m=1}^{+\infty} (\tilde{R}_j^+ R_{j-1}^-)^m \right) = R_{j-1}^+ + \frac{T_{j-1}^+ \tilde{R}_j^+ T_{j-1}^-}{1 - \tilde{R}_j^+ R_{j-1}^-}, \\ \tilde{R}_{j+1}^- &= R_{j+1}^- + T_{j+1}^- \tilde{R}_j^- T_{j+1}^+ \left( 1 + \sum_{m=1}^{+\infty} (R_{j+1}^+ \tilde{R}_j^-)^m \right) = R_{j+1}^- + \frac{T_{j+1}^- \tilde{R}_j^- T_{j+1}^+}{1 - R_{j+1}^+ \tilde{R}_j^-}, \\ \tilde{T}_{j+1}^+ &= \tilde{T}_j^+ T_{j+1}^+ \left( 1 + \sum_{m=1}^{+\infty} (R_{j+1}^+ \tilde{R}_j^-)^m \right) = \frac{\tilde{T}_j^+ T_{j+1}^+}{1 - R_{j+1}^+ \tilde{R}_j^-}, \end{aligned} \quad (52)$$

and selecting as starting the following values:

$$\tilde{R}_{N-1}^+ = R_{N-1}^+, \tilde{R}_1^- = R_1^-, \tilde{T}_1^+ = T_1^+, \quad (53)$$

we calculate successively coefficients  $\tilde{R}_{N-2}^+ \dots \tilde{R}_1^+, \tilde{R}_2^- \dots \tilde{R}_{N-1}^-$  and  $\tilde{T}_2^+ \dots \tilde{T}_{N-1}^+$ . At finishing, we determine coefficients  $\beta_j$ :

$$\beta_j = \tilde{T}_{j-1}^+ \left( 1 + \sum_{m=1}^{+\infty} (\tilde{R}_j^+ \tilde{R}_{j-1}^-)^m \right) = \frac{\tilde{T}_{j-1}^+}{1 - \tilde{R}_j^+ \tilde{R}_{j-1}^-}, \quad (54)$$

the amplitudes of transmission and reflection:

$$A_T = \tilde{T}_{N-1}^+, A_R = \tilde{R}_1^+ \quad (55)$$

and corresponding coefficients of penetrability  $T$  and reflection  $R$ :

$$T_{MIR} = \frac{k_n}{k_1} |A_T|^2, R_{MIR} = |A_R|^2. \quad (56)$$

We check the property:

$$\frac{k_n}{k_1} |A_T|^2 + |A_R|^2 = 1 \text{ or } T_{MIR} + R_{MIR} = 1, \quad (57)$$

which should be the test, whether the method MIR gives us proper solution for wave function. Now if energy of the particle is located below then height of one step with number  $m$ , then for description of transition of this particle through such barrier with its tunneling it shall need to use the following change:

$$k_m \rightarrow i \zeta_m. \quad (58)$$

For the potential from two rectangular steps (with different choice of their sizes) after comparison between the all amplitudes obtained by method of MIR and the corresponding amplitudes obtained by standard approach of quantum mechanics, we obtain coincidence up to first 15 digits. Increasing of number of steps up to some thousands keeps such accuracy and fulfillment of the property (57). This is important test which confirms reliability of the method MIR. So, we have obtained full coincidence between all amplitudes, calculated by method MIR and by standard approach of quantum mechanics, and that is way we generalize the method MIR for description of tunneling of the particle through potential, consisting from arbitrary number of rectangular barriers and wells of arbitrary shape.

### 3.4 Analysis of the proton-decay for ${}_{73}^{157}\text{Ta}$ , ${}_{75}^{161}\text{Re}$ , ${}_{77}^{167}\text{Ir}$ and ${}_{83}^{185}\text{Bi}$

Today, there are a lot of modern methods able to calculate half-lives, which have been studied experimentally well. So, we have a rich theoretical and experimental material for analysis. We shall use these nuclei:  ${}_{73}^{157}\text{Ta}$ ,  ${}_{75}^{161}\text{Re}$ ,  ${}_{77}^{167}\text{Ir}$  for  $l = 0$ , and  ${}_{53}^{109}\text{I}$ ,  ${}_{55}^{112}\text{Cm}$ ,  ${}_{69}^{147}\text{Tm}$  for  $l \neq 0$ . Such a choice we explain by that they have small coefficient of quadruple deformation  $\beta_2$  and at good approximation can be considered as spherical. We shall study proton-decay on the basis of leaving of the particle with reduced mass from the internal region outside with its tunneling through the barrier. This particle is supposed to start from  $R_{\min} \leq r \leq r_1$  and move outside ( $r_1$  is defined in eq. (1)). Using technique of the  $T_j^\pm$  and  $R_j^\pm$  coefficients in eqs. (51)–(53), we calculate total amplitudes of transmission  $A_T$  and reflection  $A_R$  by eqs. (55),

the penetrability coefficient  $T_{MIR}$  by eqs. (56). We check the found amplitudes, coefficients  $T_{MIR}$  and  $R_{MIR}$  comparing them with corresponding amplitudes and coefficients calculated by standard approach of quantum mechanics. We restrict ourselves by eq. (50) for  $F_1$  and find width  $\Gamma$  by eq. (48) and half-live  $\tau_{MIR}$  by eq. (52). We define the penetrability  $T_{WKB}$  by eq. (49), calculate  $\Gamma$ -width and half-live  $\tau_{WKB}$  by eqs. (48) and (52).

### 3.4.1 Dependence of the penetrability on the starting point

The first interesting result which we have obtained is *essential dependence of penetrability on the position of the first region where we localize the wave incident on the barrier*. In particular, we have analyzed how much the internal boundary  $R_{min}$  takes influence on the penetrability. Taking into account that width of each interval is 0.01 fm, we consider left boundary  $R_{min}$  of the first interval as a *starting point* (with error up to 0.01 fm), from here proton begins to move outside and is incident on the internal part of the barrier in the first stage of the proton decay. In the Fig. 4 [left panel] one can see that half-live of the proton decay of  $^{157}_{73}\text{Ta}$  is changed essentially at displacement of  $R_{min}$ . So, we establish *essential dependence of the penetrability on the starting point  $R_{start}$ , where the proton starts to move outside by approach MIR*. At

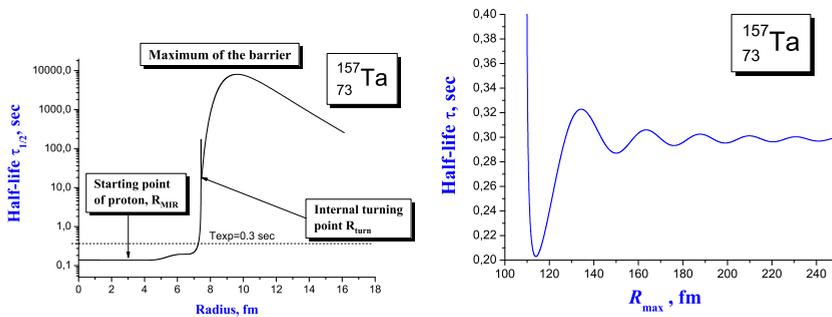


Fig. 4. Proton-decay for the  $^{157}_{73}\text{Ta}$  nucleus: the left panel is for dependence of the half-life  $\tau_{MIR}$  on the starting point  $R_{min}$ , the right panel is for dependence of the half-life  $\tau_{MIR}$  on  $R_{max}$  (here, we use  $R_{form} = 7.2127$  fm where calculated  $\tau_{MIR}$  at  $R_{max} = 250$  fm coincides with experimental data  $\tau_{exp}$  for this nucleus). In all calculations factor  $F$  is the same.

$R_{form} = 7.2127$  fm this dependence allows us to achieve very close coincidence between the half-live calculated by the approach MIR and experimental data.

### 3.4.2 Dependence of the penetrability on the external region

The region of the barrier located between turning points  $R_2$  and  $R_3$  is main part of the potential used in calculation of the penetrability in the semiclassical approach (up to the second correction), while the internal and external parts of this potential do not take influence on it. Let us analyze whether convergence exists in calculations of the penetrability in the approach MIR if to increase the external boundary  $R_{max}$  ( $R_{max} > R_3$ ). Keeping width of each interval (step) to be the same, we shall increase  $R_{max}$  (through increasing number of intervals in the external region), starting from the external turning point  $R_3$ , and calculate the corresponding penetrability  $T_{MIR}$ . In Fig. 4 [central panel] one can see how the penetrability is changed for  $^{157}_{73}\text{Ta}$  with increasing  $R_{max}$ . Dependence of the half-life  $\tau_{MIR}$  on  $R_{max}$  is shown in the next figure 4 [right panel]. One can see that the method MIR gives convergent values for the penetrability and half-life at increasing of  $R_{max}$ . From such figures we find that *inclusion of the external region into calculations changes the half-life up to 1.5 times* ( $\tau_{min} = 0.20$  sec is the

Parent nucleus				Half-live-values, sec		
Nucleus	Q, MeV	Orbit	$S_p^{\text{th}}$	$\tilde{\tau}_{WKB}$	$\tilde{\tau}_{MIR}$	$\tau_{\text{exp}}$
$^{157}_{73}\text{Ta}_{84}$	0.947	$2s_{1/2}$	0.66	$2.813 \cdot 10^{-1}$	$2.789 \cdot 10^{-1}$	$3.0 \cdot 10^{-1}$
$^{161}_{75}\text{Re}_{84}$	1.214	$2s_{1/2}$	0.59	$2.720 \cdot 10^{-4}$	$2.673 \cdot 10^{-4}$	$3.7 \cdot 10^{-4}$
$^{167}_{77}\text{Ir}_{90}$	1.086	$2s_{1/2}$	0.51	$5.85 \cdot 10^{-2}$	$5.84 \cdot 10^{-2}$	$1.1 \cdot 10^{-2}$
$^{109}_{53}\text{I}_{56}$	0.829	$1d_{5/2}$	0.76	$3.937 \cdot 10^{-6}$	$3.992 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$
$^{112}_{55}\text{Cm}_{57}$	0.823	$1d_{5/2}$	0.59	$3.526 \cdot 10^{-5}$	$3.539 \cdot 10^{-5}$	$5.0 \cdot 10^{-4}$
$^{147}_{69}\text{Tm}_{78}$	1.132	$1d_{5/2}$	0.79	$7.911 \cdot 10^{-5}$	$7.796 \cdot 10^{-5}$	$3.6 \cdot 10^{-4}$

Table 1. Experimental and calculated half-lives of some proton emitters. Here,  $S_p^{\text{th}}$  is theoretical spectroscopic factor,  $\tau_{WKB}$  is half-life calculated by in the semiclassical approach,  $\tau_{MIR}$  is half-life calculated by in the approach MIR,  $\tilde{\tau}_{WKB} = \tau_{WKB} / S_p^{\text{th}}$ ,  $\tilde{\tau}_{MIR} = \tau_{MIR} / S_p^{\text{th}}$ ,  $\tau_{\text{exp}}$  is experimental data. Values for  $S_p^{\text{th}}$ ,  $\tau_{\text{exp}}$  are used from Table IV in Ref. (Aberg et al., 1997) (see p. 1770); in calculations for each nucleus we use:  $R_{\text{min}} = 0.11$  fm,  $R_{\text{max}} = 250$  fm; number of intervals in region from  $R_{\text{min}}$  to maximum of the barrier is 10000, from maximum of the barrier to  $R_{\text{max}}$  is 10000.

minimal half-life calculated at  $R_3 \leq R_{\text{max}} \leq 250$  fm,  $\tau_{\text{as}} = 0.30$  sec is the half-life calculated at  $R_{\text{max}} = 250$  fm, error =  $\tau_{\text{as}} / \tau_{\text{min}} \approx 1.5$  or 50 percents). So, *error in determination of the penetrability in the semiclassical approach (if to take the external region into account) is expected to be the same as a minimum on such a basis.*

### 3.4.3 Results of calculations of half-lives in our and semiclassical approaches

As we have demonstrated above, the fully quantum calculations of the penetrability of the barrier for the proton decay give us its essential dependence on the starting point. In order to give power of predictions of half-lives calculated by the approach MIR, we need to find recipe able to resolve such uncertainty in calculations of the half-lives. So, we shall introduce the following hypothesis: *we shall assume that in the first stage of the proton decay proton starts to move outside the most probably at the coordinate of minimum of the internal well.* If such a point is located in the minimum of the well, the penetrability turns out to be maximal and half-life minimal. So, as criterion we could use minimum of half-live for the given potential, which has stable basis. We should take into account that the half-lives obtained before are for the proton occupied ground state while it needs to take into account probability that this state is empty in the daughter nucleus. In order to obtain proper values for the half-lives we should divide them on the spectroscopic factor  $S$  (which we take from (Aberg et al., 1997)), and then to compare them with experimental data. Results of such calculations and experimental data for some proton emitters are presented in Table 1. To complete a picture, we add half-lives calculated by the semiclassical approach to these data.

## 4. On four-position operators in quantum field theory, in terms of bilinear operators

In this Section we approach the *relativistic* case, taking into consideration — therefore — the space-time (four-dimensional) “position” operator, starting however with an analysis of the 3-dimensional (spatial) position operator in the simple relativistic case of the Klein-Gordon equation. Actually, this analysis will lead us to tackle already with non-hermitian operators.

Moreover, while performing it, we shall meet the opportunity of introducing bilinear operators, which will be used even more in the next case of the full 4-position operator.

Let us recall that in Sect.2.1 we mentioned that the boundary condition  $E \neq 0$ , therein imposed to guarantee (maximal) hermiticity of the time operator, can be dispensed with just by having recourse to bilinear forms. Namely, by considering the bilinear hermitian operator (Recami, 1976; 1977; Recami et al., 1983)  $\hat{t} = (-i\hbar \overset{\leftrightarrow}{\partial} / \partial E) / 2$ , where the sign  $\leftrightarrow$  is defined through the accompanying equality  $(f, \hat{t}g) = \left(f, -\frac{i\hbar}{2} \frac{\partial}{\partial E} g\right) + \left(-\frac{i\hbar}{2} \frac{\partial}{\partial E} f, g\right)$ .

#### 4.1 The Klein-Gordon case: Three-position operators

The standard position operators, being hermitian and moreover selfadjoint, are known to possess real eigenvalues: i.e., they yield a *point-like* localization. J. M. Jauch showed, however, that a point-like localization would be in contrast with “unimodularity”. In the relativistic case, moreover, phenomena so as the pair production forbid a localization with precision better than one Compton wave-length. The eigenvalues of a realistic position operator  $\hat{z}$  are therefore expected to represent space *regions*, rather than points. This can be obtained only by having recourse to non-hermitian (and therefore non-selfadjoint) position operators  $\hat{z}$  (a priori, one can have recourse either to non-normal operators with commuting components, or to normal operators with non-commuting components). Following, e.g., the ideas in Ref. (Gallardo et al., 1967b;c; Ka’lnay, 1966; Ka’lnay & Toledo, 1967; Olkhovsky et al., 1967), we are going to show that the mean values of the *hermitian (selfadjoint) part* of  $\hat{z}$  will yield a mean (point-like) position (Baldo & Recami, 1969; Recami, 1970), while the mean values of the *anti-hermitian (anti-selfadjoint) part* of  $\hat{z}$  will yield the sizes of the localization region (Olkhovsky & Recami, 1968; 1969).

Let us consider, e.g., the case of relativistic spin-zero particles, in natural units and with metric  $(+ - - -)$ . The position operator  $i \nabla_{\mathbf{p}}$ , is known to be actually non-hermitian, and may be in itself a good candidate for an extended-type position operator. To show this, we want to split (Gallardo et al., 1967b;c; Ka’lnay, 1966; Ka’lnay & Toledo, 1967; Olkhovsky et al., 1967) it into its hermitian and anti-hermitian (or skew-hermitian) parts.

Consider, then, a vector space  $V$  of complex differentiable functions on a 3-dimensional phase-space (Recami et al., 1983) equipped with an inner product defined by

$$(\Psi, \Phi) = \int \frac{d^3 \mathbf{p}}{p_0} \Psi^*(\mathbf{p}) \Phi(\mathbf{p}) \quad (59)$$

quantity  $p_0$  being  $\sqrt{\mathbf{p}^2 + m_0^2}$ . Let the functions in  $V$  satisfy moreover the condition

$$\lim_{R \rightarrow \infty} \int_{S_R} \frac{dS}{p_0} \Psi^*(\mathbf{p}) \Phi(\mathbf{p}) = 0 \quad (60)$$

where the integral is taken over the surface of a sphere of radius  $R$ . If  $U : V \rightarrow V$  is a differential operator of degree one, condition (60) allows a definition of the transpose  $U^T$  by

$$(U^T \Psi, \Phi) = (\Psi, U \Phi) \text{ for all } \Psi, \Phi \in V, \quad (61)$$

where  $U$  is changed into  $U^T$ , or vice-versa, by means of integration by parts.

This allows, further, to introduce a *dual representation* (Recami et al., 1983) ( $U_1, U_2$ ) of a *single* operator  $U_1^T + U_2$  by

$$(U_1\Psi, \Phi) + (\Psi, U_2\Phi) = (\Psi, (U_1^T + U_2)\Phi). \quad (62)$$

With such a dual representation, it is easy to split any operator into its hermitian and anti-hermitian parts

$$(\Psi, U\Phi) = \frac{1}{2} \left( (\Psi, U\Phi) + (U^*\Psi, \Phi) \right) + \frac{1}{2} \left( (\Psi, U\Phi) - (U^*\Psi, \Phi) \right). \quad (63)$$

Here the pair

$$\frac{1}{2} (U^*, U) \equiv \overset{\leftrightarrow}{U}_h, \quad (64)$$

corresponding to  $(1/2) (U + U^{*T})$ , represents the hermitian part, while

$$\frac{1}{2} (-U^*, U) \equiv \overset{\leftrightarrow}{U}_a \quad (65)$$

represents the anti-hermitian part.

Let us apply what precedes to the case of the Klein-Gordon position-operator  $\hat{z} = i \nabla_p$ . When

$$U = i \frac{\partial}{\partial p_j} \quad (66)$$

we have (Olkhovsky & Recami, 1968; 1969)

$$\begin{aligned} \frac{1}{2} (U^*, U) &= \frac{1}{2} \left( -i \frac{\partial}{\partial p_j}, i \frac{\partial}{\partial p_j} \right) \equiv \frac{i}{2} \overset{\leftrightarrow}{\frac{\partial}{\partial p_j}}, \quad (a) \\ \frac{1}{2} (-U^*, U) &= \frac{1}{2} \left( i \frac{\partial}{\partial p_j}, i \frac{\partial}{\partial p_j} \right) \equiv \frac{i}{2} \overset{\leftrightarrow}{\frac{\partial}{\partial p_j}}. \quad (b) \end{aligned} \quad (67)$$

And the corresponding *single* operators turn out to be

$$\begin{aligned} \frac{1}{2} (U + U^{*T}) &= i \frac{\partial}{\partial p_j} - \frac{i}{2} \frac{p_j}{p^2 + m_0^2}, \quad (a) \\ \frac{1}{2} (U - U^{*T}) &= \frac{i}{2} \frac{p_j}{p^2 + m_0^2}. \quad (b) \end{aligned} \quad (68)$$

It is noteworthy (Olkhovsky & Recami, 1968; 1969) that, as we are going to see, operator (68a) is nothing but the usual Newton-Wigner operator, while (68b) can be interpreted (Gallardo et al., 1967b;c; Ka'lnay, 1966; Ka'lnay & Toledo, 1967; Olkhovsky et al., 1967; Olkhovsky & Recami, 1968; 1969; Toller, 1999) as yielding the sizes of the localization-region (an ellipsoid) via its average values over the considered wave-packet.

Let us underline that the previous formalism justifies from the mathematical point of view the treatment presented in papers like (Baldo & Recami, 1969; Gallardo et al., 1967b;c; Ka'lnay, 1966; Ka'lnay & Toledo, 1967; Olkhovsky et al., 1967; Recami, 1970). We can split (Olkhovsky & Recami, 1968; 1969) the operator  $\hat{z}$  into two *bilinear* parts, as follows:

$$\hat{z} = i \nabla_p = \frac{i}{2} \overset{\leftrightarrow}{\nabla}_p + \frac{i}{2} \overset{\leftrightarrow(+)}{\nabla}_p \quad (69)$$

where  $\Psi^* \overset{\leftrightarrow}{\nabla}_p \Phi \equiv \Psi^* \nabla_p \Phi - \Phi \nabla_p \Psi^*$  and  $\Psi^* \overset{\leftrightarrow(+)}{\nabla}_p \Phi \equiv \Psi^* \nabla_p \Phi + \Phi \nabla_p \Psi^*$ , and where we always referred to a suitable (Baldo & Recami, 1969; Gallardo et al., 1967b;c; Ka'lnay, 1966; Ka'lnay & Toledo, 1967; Olkhovsky et al., 1967; Recami, 1970; 1976; 1977; Recami et al., 1983) space of wave packets. Its hermitian part (Baldo & Recami, 1969; Gallardo et al., 1967b;c; Ka'lnay, 1966; Ka'lnay & Toledo, 1967; Olkhovsky et al., 1967; Recami, 1970)

$$\hat{x} = \frac{i}{2} \overset{\leftrightarrow}{\nabla}_p, \quad (70)$$

which was expected to yield an (ordinary) point-like localization, has been derived also by writing explicitly

$$(\Psi, \hat{x} \Phi) = i \int \frac{d^3 p}{p_0} \Psi^*(p) \nabla_p \Phi(p) \quad (71)$$

and imposing hermiticity, i.e., imposing the reality of the diagonal elements. The calculations yield

$$\Re(\Phi, \hat{x} \Phi) = i \int \frac{d^3 p}{p_0} \Phi^*(p) \overset{\leftrightarrow}{\nabla}_p \Phi(p), \quad (72)$$

suggesting to adopt just the Lorentz-invariant quantity (70) as a bilinear hermitian position operator. Then, on integrating by parts (and due to the vanishing of the surface integral), we verify that eq. (70) is equivalent to the ordinary Newton-Wigner operator:

$$\hat{x}_h \equiv \frac{i}{2} \overset{\leftrightarrow}{\nabla}_p \equiv i \nabla_p - \frac{i}{2} \frac{\mathbf{p}}{p^2 + m^2} \equiv \mathbf{N} - \mathbf{W}. \quad (73)$$

We are left with the (bilinear) anti-hermitian part

$$\hat{y} = \frac{i}{2} \overset{\leftrightarrow(+)}{\nabla}_p \quad (74)$$

whose *average values* over the considered state (wave-packet) can be regarded as yielding (Baldo & Recami, 1969; Gallardo et al., 1967b;c; Ka'lnay, 1966; Ka'lnay & Toledo, 1967; Olkhovsky et al., 1967; Recami, 1970; 1976; 1977; Recami et al., 1983) the sizes of an ellipsoidal localization-region.

After the digression associated with eqs.(69)–(74), let us go back to the present formalism, as expressed by eqs.(59)–(68).

In general, the extended-type position operator  $\hat{z}$  will yield

$$\langle \Psi | \hat{z} | \Psi \rangle = (\alpha + \Delta\alpha) + i(\beta + \Delta\beta), \quad (75)$$

where  $\Delta\alpha$  and  $\Delta\beta$  are the mean-errors encountered when measuring the point-like position and the sizes of the localization region, respectively. It is interesting to evaluate the commutators ( $i, j = 1, 2, 3$ ):

$$\left( \frac{i}{2} \overset{\leftrightarrow}{\frac{\partial}{\partial p_i}}, \frac{i}{2} \overset{\leftrightarrow(+)}{\frac{\partial}{\partial p_j}} \right) = \frac{i}{2 p_0^2} \left( \delta_{ij} - \frac{2 p_i p_j}{p_0^2} \right), \quad (76)$$

wherefrom the noticeable “uncertainty correlations” follow:

$$\Delta\alpha_i \Delta\beta_j \geq \frac{1}{4} \left| \left\langle \frac{1}{p_0^2} \left( \delta_{ij} - \frac{2 p_i p_j}{p_0^2} \right) \right\rangle \right|. \quad (77)$$

## 4.2 Four-position operators

It is tempting to propose as *four-position operator* the quantity  $\hat{z}^\mu = \hat{x}^\mu + i\hat{y}^\mu$ , whose hermitian (Lorentz-covariant) part can be written

$$\hat{x}^\mu = -\frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial p_\mu}, \quad (78)$$

to be associated with its corresponding “operator” in four-momentum space

$$\hat{p}_h^\mu = +\frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial x_\mu}. \quad (79)$$

Let us recall the proportionality between the 4-momentum operator and the 4-current density operator in the chronotopical space, and then underline the canonical correspondence (in the 4-position and 4-momentum spaces, respectively) between the “operators” (cf. the previous subsection):

$$m_0 \hat{p} \equiv \hat{p}_0 = \frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial t} \quad (a)$$

$$m_0 \hat{j} \equiv \hat{p} = -\frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial \mathbf{r}}, \quad (b)$$

and the operators

$$\hat{t} \equiv -\frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial p_0} \quad (a)$$

$$\hat{x} \equiv \frac{i}{2} \frac{\overleftrightarrow{\partial}}{\partial \mathbf{p}}, \quad (b)$$

where the four-position “operator” (81) can be considered as a 4-current density operator in the energy-impulse space. Analogous considerations can be carried on for the anti-hermitian parts (see the last one of Refs.(Olkhovsky & Recami, 1968; 1969)).

Finally, by recalling the properties of the time operator as a maximal hermitian operator in the non-relativistic case (Sec.2.1), one can see that the relativistic time operator (81a) (for the Klein-Gordon case) is also a selfadjoint bilinear operator for the case of continuous energy spectra, and a (maximal) hermitian linear operator for free particles [due to the presence of the lower limit zero for the kinetic energy, or  $m_0$  for the total energy].

## 5. Decoherence (without instantaneous wave-function collapse<sup>5</sup>)

In this paper we want to show, within the density matrix formalism, that a simple way to get decoherence is through the introduction of a “quantum” of time (or rather of a *chronon*): thus replacing the differential Liouville–von Neumann equation with a finite-difference version of it. In this way, one is given the possibility of using a very simple quantum equation to describe the decoherence effects due to dissipation, and of partially solving the measurement-problem in quantum mechanics (avoiding any recourse to the wave-function collapse). *Namely*, the mere introduction (not of a “time-lattice”, but simply) of the “chronon” allows us to go on from differential to finite-difference equations; and in particular to write down the

<sup>5</sup> This section is developed by Erasmo Recami.

Schrödinger equation (as well as the Liouville–von Neumann equation) in three different ways: “retarded”, “symmetrical”, and “advanced”. One of such three formulations — the *retarded* one — describes in an elementary way a system which is exchanging (and losing) energy with the environment. In its density-matrix version, indeed, it can be easily shown that all non-diagonal terms go to zero very rapidly.

Let us refer, in particular, to the theory of the *chronon* as proposed by P. Caldirola. Let us recall that such an interesting “finite difference” theory, forwards — at the classical level — a solution for the motion of a particle endowed with a non-negligible charge in an external electromagnetic field, overcoming all the known difficulties met by Abraham-Lorentz’s and Dirac’s approaches (and even allowing a clear answer to the question whether a free falling charged particle does or does not emit radiation), and — at the quantum level — yields a remarkable mass spectrum for leptons.

It is easy to compare one another the *new* representations of Quantum Mechanics (QM) resulting from it, in the Schrödinger, Heisenberg and density operator (Liouville–von Neumann) pictures, respectively.

For each representation, three (*retarded*, *symmetric* and *advanced*) formulations are possible, which refer either to times  $t$  and  $t - \tau_0$ , or to times  $t - \tau_0/2$  and  $t + \tau_0/2$ , or to times  $t$  and  $t + \tau_0$ , respectively. It is interesting to notice that, when the chronon tends to zero, the ordinary QM is obtained as the limiting case of the “symmetric” formulation only; while the “retarded” one does naturally appear to describe QM with friction, i. e., to describe *dissipative* quantum systems (like a particle moving in an absorbing medium).

In this sense, *discretized* QM is much richer than the ordinary one. Here, we want to pay attention to the fact that, when applying the density matrix formalism to the solution of the *measurement problem* in QM, interesting results are met, as, for instance, a natural explication of the “decoherence” due to dissipation: which seem to reveal the power of discretized (in particular, *retarded*) QM.

### 5.1 On discretized Quantum Mechanics

Let us approach our eventual application of the discretization procedures for a possible solution of the measurement problem in Quantum Mechanics, without having to make recourse to the reduction (wave-packet instantaneous collapse) postulate. Namely, let us focus our attention, now, on the consequences for QM of the introduction of a chronon. In QM, time will still be a continuous variable, but the evolution of the system along its world line will be regarded as discontinuous. In analogy with the electron theory in the *non-relativistic* limit, one has to substitute the corresponding finite-difference expression for the time derivatives; e. g.:

$$\frac{df(t)}{dt} = \frac{f(t) - f(t - \Delta t)}{\Delta t}, \quad (82)$$

where proper time is now replaced by the local time  $t$ . The chronon procedure can then be applied to obtain the finite-difference form of the Schrödinger equation. As for the electron case, there are three different ways to perform the discretization, and three “Schrödinger equations” can be obtained:

$$i \frac{\hbar}{\tau} [\Psi(x, t) - \Psi(x, t - \tau)] = \hat{H} \Psi(x, t), \quad (83)$$

$$i \frac{\hbar}{2\tau} [\Psi(x, t + \tau) - \Psi(x, t - \tau)] = \hat{H} \Psi(x, t), \quad (84)$$

$$i \frac{\hbar}{\tau} [\Psi(x, t + \tau) - \Psi(x, t)] = \hat{H} \Psi(x, t), \quad (85)$$

which are, respectively, the *retarded*, *symmetric* and *advanced* Schrödinger equations, all of them transforming into the (same) continuous equation when the fundamental interval of time (that can now be called just  $\tau$ ) goes to zero.

Since the equations are different, the solutions they provide are also fundamentally different. In the classical theory of the electron the symmetric equation represented a non-radiating motion, providing only an approximate description of the motion (without taking into account the effects due to the self fields of the electron). However, in the quantum theory it plays a fundamental role. In the discrete formalism too, the symmetrical equation constitutes the only way to describe a bound non-radiating particle.

However, the solutions of the *retarded* (and *advanced*) equations show a completely different behaviour. For a Hamiltonian explicitly independent of time, the solutions have a general form given by

$$\Psi(x, t) = \left[ 1 + i \frac{\tau}{\hbar} \hat{H} \right]^{-t/\tau} f(x) \quad (86)$$

and, expanding  $f(x)$  in terms of the eigenfunctions of  $\hat{H}$ :

$$\hat{H} u_n(x) = W_n u_n(x), \quad (87)$$

that is, writing  $f(x) = \sum_n c_n u_n(x)$ , with  $\sum_n |c_n|^2 = 1$ , one can obtain that

$$\Psi(x, t) = \sum_n c_n \left[ 1 + i \frac{\tau}{\hbar} W_n \right]^{-t/\tau} u_n(x). \quad (88)$$

The norm of this solution is given by

$$|\Psi(x, t)|^2 = \sum_n |c_n|^2 \exp(-\gamma_n t) \quad (89)$$

with

$$\gamma_n = \frac{1}{\tau} \ln \left( 1 + \frac{\tau^2}{\hbar^2} W_n^2 \right) = \frac{W_n^2}{\hbar^2} \tau + O(\tau^3), \quad (90)$$

where it is apparent that the damping factor depends critically on the value  $\tau$  of the chronon. This *dissipative* behaviour originates from the character of the *retarded* equation; in the case of the electron, the retarded equation possesses intrinsically dissipative solutions, representing a radiating system. The Hamiltonian has the same status as in the ordinary (continuous) case: It is an observable, since it is a hermitian operator and its eigenvectors form a basis of the state space. However, as we have seen, the norm of the state vector is not constant any longer, due to the damping factor. An opposite behaviour is observed for the solutions of the advanced equation, in the sense that they increase exponentially.

## 5.2 Discretized (retarded) Liouville equation, and a solution of the measurement problem: Decoherence from dissipation

Suppose we want to measure the dynamical variable  $R$  of a (microscopic) object  $\mathcal{O}$ , by utilizing a (macroscopic) measuring apparatus  $\mathcal{A}$ .

In the discrete case the interaction is embedded in the Hamiltonian  $\hat{H}$ , with the following consequences. Let us consider the energy representation, where  $|n\rangle$  are the states with defined

energy:  $H|n\rangle = E_n|n\rangle$ . Since the time evolution operator is a function of the Hamiltonian, and commutes with it, the basis of the energy eigenstates will be a basis also for this operator. The discretized (retarded) Liouville-von Neumann equation is

$$\frac{\rho(t) - \rho(t - \tau)}{\tau} = -i\mathcal{L}\rho(t), \quad (91)$$

which reduces to the LvN equation when  $\tau \rightarrow 0$ . The essential point is that, following e.g. a procedure similar to Bonifacio's, one gets in this case a *non-unitary* time-evolution operator:

$$V(t, 0) = \left[ 1 + \frac{i\tau\mathcal{L}}{\hbar} \right]^{-t/\tau}, \quad (92)$$

which, as all non-unitary operators, does not preserve the probabilities associated with each of the energy eigenstates (that make up the expansion of the initial state in such a basis of eigenstates). We are interested in the time instants  $t = k\tau$ , with  $k$  an integer.

Thus, the time-evolution operator (92) takes the initial density operator  $\rho^{\text{in}}$  to a final state for which the non-diagonal terms decay exponentially with time; namely, to

$$\rho_{rs}^{\text{fin}} = \langle r|V(t, 0)|s\rangle = \rho_{rs}^{\text{in}} [1 + iw_{rs}\tau]^{-t/\tau}, \quad (93)$$

where

$$w_{rs} \equiv \frac{1}{\hbar} (E_r - E_s) \equiv \frac{1}{\hbar} (\Delta E)_{rs}. \quad (94)$$

Expression (93) can be written

$$\rho_{rs}(t) = \rho_{rs}(0) e^{-\gamma_{rs}t} e^{-iv_{rs}t}, \quad (95)$$

with

$$\gamma_{rs} \equiv \frac{1}{2\tau} \ln(1 + w_{rs}^2\tau^2), \quad (96)$$

$$v_{rs} \equiv \frac{1}{\tau} \tan^{-1}(w_{rs}\tau). \quad (97)$$

One can observe, indeed, that the non-diagonal terms tend to zero with time, and that the larger the value of  $\tau$ , the faster the decay becomes. Actually, the chronon  $\tau$  is now an interval of time related no longer to a single electron, but to the whole system  $\mathcal{O} + \mathcal{A}$ . If one imagines the time interval  $\tau$  to be linked to the possibility of distinguishing two successive, different states of the system, then  $\tau$  can be significantly larger than  $10^{-23}$  sec, implying an extremely faster damping of the non-diagonal terms of the density operator.

Thus, the reduction to the diagonal form occurs, provided that  $\tau$  possesses a finite value, no matter how small, and provided that  $w_{nm}\tau$ , for every  $n, m$ , is not much smaller than 1; where

$$w_{nm} = (E_n - E_m)/\hbar \quad (98)$$

are the transition frequencies between the different energy eigenstates (the last condition being always satisfied, e. g., for non-bounded systems).

It is essential to notice that *decoherence has been obtained above, without having recourse to any statistical approach, and in particular without assuming any "coarse graining" of time*. The reduction to the diagonal form illustrated by us is a consequence of the discrete (retarded) Liouville-von Neumann equation only, once the inequality  $w_{nm}\tau \ll 1$  is *not* verified.

Moreover, the measurement problem is still controversial even with regard to its mathematical approach: In the simplified formalization introduced above, however, we have not included any consideration beyond those common to the quantum formalism, allowing an as clear as possible recognition of the effects of the introduction of a chronon.

## 6. Non-hermitian Hamiltonians and microscopic quantum dissipation

Various different approaches are known, aimed at getting dissipation — and possibly decoherence — within quantum mechanics. First of all, the simple introduction of a “chronon” (see, e.g., Refs. (Caldirola et al., 1978; Caldirola, 1979; Caldirola & Montaldi, 1979; Caldirola & Lugiato, 1982; Caldirola, 1983; Farias & Recami, 2007)) allows one to go on from differential to finite-difference equations, and in particular to write down the quantum theoretical equations (Schrödinger’s, Liouville-von Neumann’s, etc.) in three different ways: symmetrical, retarded, and advanced. The retarded “Schrödinger” equation describes in a rather simple and natural way a dissipative system, which exchanges (loses) energy with the environment. The corresponding non-unitary time-evolution operator obeys a semigroup law and refers to irreversible processes. The retarded approach furnishes, moreover, an interesting way for solving the “measurement problem” in quantum mechanics, without any need for a wave-function collapse: see Refs. (Bonifacio, 1983; Bonifacio & Caldirola, 1983; Farias & Recami, 2007; Ghirardi & Weber, 1984; Recami & Farias, 2002). The chronon theory can be regarded as a peculiar “coarse grained” description of the time evolution.

Let us stress that it has been shown that the mentioned discrete approach can be replaced with a continuous one, at the price of introducing a *non-hermitian* Hamiltonian: see, e.g., Ref. (Casagrande & Montaldi, 1977).

Further relevant work can be found, for instance, in papers like (Caldirola, 1941; Janussis et al., 1980; 1981a;b; 1982a;b;c; 1984; 1991; 1995; Mignani, 1983) and refs. therein.

Let us add, at this point, that much work is still needed for the description of time irreversibility at the microscopic level. Indeed, various approaches have been proposed, in which new parameters are introduced (regulation or dissipation) into the microscopic dynamics (building a bridge, in a sense, between microscopic structure and macroscopic characteristics). Besides the Caldirola-Kanai (Caldirola, 1941; Kanai, 1948) Hamiltonian

$$\hat{H}_{CK}(t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} e^{-\gamma t} + V(x) e^{\gamma t} \quad (99)$$

(which has been used, e.g., in Ref. (Angelopoulos et al., 1995)), other rather simple approaches, based of course on the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{H} \Psi(x, t), \quad (100)$$

and adopting a microscopic dissipation defined via a coefficient of extinction  $\gamma$ , are for instance the following ones:

A) *Non-linear (non-hermitian) Hamiltonians*

$$\hat{H}_{nl} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) + \hat{W}, \quad (101)$$

with “potential” operators  $\hat{W}$  of the type:

1. Kostin’s operator (see Ref. (Kostin, 1972)):

$$\hat{W}_K = -\frac{i\hbar}{2m} \left\{ \frac{\ln \Psi}{\Psi^*} - \left\langle \frac{\ln \Psi}{\Psi^*} \right\rangle \right\}; \quad (102)$$

2. Albrecht's operator (see Ref.(Albrecht, 1975)):

$$\hat{W}_A(x) = \langle p \rangle (x - \langle x \rangle), \quad (103)$$

where  $\langle \rangle$  is the averaging produced over  $|\Psi(x)|^2$ ;

3. Ref.(Hasse, 1975):

$$\hat{W}_H(x) = \frac{1}{4} [x - \langle x \rangle, p + \langle p \rangle]_+, \quad (104)$$

where  $[A, B]_+$  is the anticommutator:  $[A, B]_+ = AB + BA$ .

#### B) Linear (non-hermitian) Hamiltonians:

1. Ref.(Gisin, 1982):

$$\hat{H}_G = (1 - i\gamma) \hat{H} + i\gamma \langle \hat{H} \rangle; \quad (105)$$

2. Ref.(Exner, 1983):

$$\hat{H}_E = \hat{H} + i\hat{W}(x) - i\langle \hat{W}(x) \rangle. \quad (106)$$

One might recall also the important, so-called "microscopic models"(Caldeira & Leggett, 1983), even if they are not based on the Schrödinger equation.

All such proposals are to be further investigated, and completed, since they have not been apparently exploited enough, till now. Let us remark, just as an example, that it would be desirable to take into deeper consideration other related phenomena, like the ones associated with the "Hartman effect" (and "generalized Hartman effect") (Aharonov, 2002; Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; 2002; 2004; 2005; Recami, 2004), in the case of tunneling with dissipation: a topic faced in few papers, like (Nimtz et al., 1994; Raciti & Salesi, 1994).

As a small contribution of ours, in the Appendix we present a scheme of iterations (successive approximations) as a possible tool for explicit calculations of wave-functions in the presence of dissipation, by using as an example the simple Albrecht's potential. Our scheme may be useful, in any case, for the investigation of possible violations of the Hartman effect, as well as for analyzing a few irreversible phenomena. See the Appendix.

At last, let us incidentally recall that two generalized Schrödinger equations, introduced by Caldirola (Caldirola, 1941; 1976a;b; 1977) in order to describe two different dissipative processes (behavior of open systems, and the radiation of a charged particle) have been shown — see, e.g., Ref.(Mignani, 1983)) — to possess the same algebraic structure of the Lie-admissible type(Santilli, 1983).

## 7. Some conclusions

1. We have shown that the Time operator (1), hermitian even if non-selfadjoint, works for any quantum collisions or motions, in the case of a continuum energy spectrum, in non-relativistic quantum mechanics and in one-dimensional quantum electrodynamics. The uniqueness of the (maximal) hermitian time operator (1) directly follows from the uniqueness of the Fourier-transformations from the time to the energy representation. The time operator (1) has been fruitfully used in the case, for instance, of tunnelling times (see Refs. (Olkhovsky & Recami, 1992; Olkhovsky et al., 1995; Olkhovsky & Agresti, 1997; Olkhovsky et al., 2004; Olkhovsky & Recami, 2007)), and of nuclear reactions and decays (see Refs. (Olkhovsky, 1984; 1990; 1992; 1998) and also Ref. (Olkhovsky et al., 2006)). We have discussed the advantages of such an approach with respect to POVM's, which is not applicable for three-dimensional particle collisions, within a wide class of Hamiltonians.

The mathematical properties of the present Time operator have actually demonstrated — without introducing any new physical postulates — that *time* can be regarded as a quantum-mechanical observable, at the same degree of other physical quantities (energy, momentum, spatial coordinates,...).

The commutation relations (eqs. (8), (22), (31)) here analyzed, and the uncertainty relations (9), result to be analogous to those known for other pairs of canonically conjugate observables (as for coordinate  $\hat{x}$  and momentum  $\hat{p}_x$ , in the case of eq. (9)). Of course, our new relations do not replace, but merely extend the meaning of the classic time and energy uncertainties, given e.g. in Ref. (Olkhovsky & Recami, 2008). In subsection 2.6, we have studied the properties of Time, as an observable, for quantum-mechanical systems with *discrete* energy spectra.

2. Let us recall that the Time operator (1), and relations (2), (3), (4), (15), (16), have been used for the temporal analysis of nuclear reactions and decays in Refs. (Olkhovsky, 1984; 1990; 1992; 1998); as well as of new phenomena, about time delays-advances in nuclear physics and about time resonances or explosions of highly excited compound nuclei, in Refs. (D'Arrigo et al., 1992; 1993; Olkhovskiy & Doroshko, 1992; Olkhovskiy et al., 2006). Let us also recall that, besides the time operator, other quantities, to which (maximal) hermitian operators correspond, can be analogously regarded as quantum-physical observables: For example, von Neumann himself (Recami, 1976; 1977; Von Neumann, 1955)) considered the case of the momentum operator  $-i\partial/\partial x$  in a semi-space with a rigid wall orthogonal to the  $x$ -axis at  $x = 0$ , or of the radial momentum  $-i\partial/\partial r$ , even if both act on packets defined only over the positive  $x$  or  $r$  axis, respectively.

Subsection 2.5 has been devoted to a new “hamiltonian approach”: namely, to the introduction of the analogue of the “Hamiltonian” for the case of the Time operator.

3. In Section 3, we have proposed a suitable generalization for the Time operator (or, rather, for a Space-Time operator) in relativistic quantum mechanics. For instance, for the Klein-Gordon case, we have shown that the hermitian part of the three-position operator  $\hat{x}$  is nothing but the Newton-Wigner operator, and corresponds to a point-like position; while its anti-hermitian part can be regarded as yielding the sizes of an extended-type (ellipsoidal) localization. When dealing with a 4-position operator, one finds that the Time operator is selfadjoint for unbounded energy spectra, while it is a (maximal) hermitian operator when the kinetic energy, and the total energy, are bounded from below, as for a free particle. We have extensively made recourse, in the latter case, to *bilinear* forms, which dispense with the necessity of eliminating the lower point — corresponding to zero velocity — of the spectra. It would be interesting to proceed to further generalizations of the 3- and 4-position operator for other relativistic cases, and analyze the localization problems associated with Dirac particles, or in 2D and 3D quantum electrodynamics, etc. Work is in progress on time analyses in 2D quantum electrodynamic, for application, e.g., to frustrated (almost total) internal reflections. Further work has still to be done also about the joint consideration of particles and antiparticles.

4. Section 4 has been devoted to the association of unstable states (decaying “resonances”) with the eigenvectors of quasi-hermitian (Agodi et al., 1973; Olkhovskiy et al., 2006; Recami et al., 1983) Hamiltonians.

5. Non-hermitian Hamiltonians, and non-unitary time-evolution operators, can play an important role also in microscopic quantum dissipation (Bonifacio, 1983; Bonifacio & Caldirola, 1983; Caldirola, 1941; Caldirola et al., 1978; Caldirola, 1979; Caldirola & Montaldi, 1979; Caldirola & Lugiato, 1982; Caldirola, 1983; Casagrande & Montaldi, 1977; Farias & Recami, 2007; Ghirardi & Weber, 1984; Janussis et al., 1980; 1981a,b; 1982a,b,c; 1984; 1991; 1995; Mignani, 1983; Recami & Farias, 2002): namely, in getting decoherence through interaction

with the environment (Farias & Recami, 2007; Recami & Farias, 2002). This topic is touched in Section 5; together with questions related with collisions in absorbing media. In particular, in Sec.5 we mention also the case of the optical model in nuclear physics; without forgetting that non-hermitian operators show up even in the case of tunnelling — e. g., in fission phenomena — with quantum dissipation, and of quantum friction. As to the former topic of microscopic quantum dissipation, among the many approaches to quantum irreversibility we have discussed in Sec. 5.2 a possible solution of the quantum measurement problem (via interaction with the environment) by the introduction of finite-difference equations (e. g., in terms of a “chronon”).

6. Let us eventually observe that the “dual equations” (26) and (27) seem to be promising also for the study the initial stage of our cosmos, when tunnellings can take place through the barriers which appear in quantum gravity in the limiting case of quasi-Schrödinger equations.

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## 9. Appendix

### Time-dependent Schrödinger equation with dissipative terms

#### 9.1 Introduction

Let's consider the time-dependent Schrödinger equation:

$$i \frac{\partial}{\partial t} \Psi(x, t) = \left( -\frac{\partial^2}{\partial x^2} + V(x, t) \right) \Psi(x, t), \quad (107)$$

where we put  $\hbar = 1$ . Let us rewrite the time-dependent wave function (WF),  $\Psi(x, t)$  (which can be considered as a wave-packet (WP)), in the form of a Fourier integral:

$$\Psi(x, t) = \int_0^{E_0} g(E) e^{-iEt} \varphi(E, x) dE, \quad (108)$$

where  $\varphi(E, x)$  is the WF component independent of time, and  $g(E)$  is a weight factor. One can choose the function  $g(E)$  to be, e.g., a *Gaussian*:

$$g(E) = A e^{-a^2(k-\bar{k})^2}. \quad (109)$$

Here,  $A$  and  $a$  are constants, and  $\bar{k}$  is the selected value for the impulse, constituting the center of the WP. We substitute the Fourier-expansion (108) of WF into eq. (107). Thus, the l.h.s. of this equation transforms into

$$i \frac{\partial}{\partial t} \Psi(x, t) = \int_0^{E_0} g(E) e^{-iEt} \varphi(E, x) E dE. \quad (110)$$

Afterwards, the r.h.s. of eq. (107) gets transformed into

$$\left(-\frac{\partial^2}{\partial x^2} + V(x, t)\right) \Psi(x, t) = -\int_0^{E_0} g(E) e^{-iEt} \frac{\partial^2 \varphi(E, x)}{\partial x^2} dE + \int_0^{E_0} g(E) V(x, \bar{E}, t) e^{-iEt} \varphi(E, x) dE. \quad (111)$$

Therefore, the whole equation (107) has been transformed into

$$\int_0^{E_0} g(E) e^{-iEt} \varphi(E, x) E dE = -\int_0^{E_0} g(E) e^{-iEt} \frac{\partial^2 \varphi(E, x)}{\partial x^2} dE + \int_0^{E_0} g(E) V(x, \bar{E}, t) e^{-iEt} \varphi(E, x) dE. \quad (112)$$

Let us now apply the inverse Fourier-transformation to this equation. Its left part becomes

$$\begin{aligned} \frac{1}{2\pi} \int dt e^{iE't} \int_0^{E_0} g(E) e^{-iEt} \varphi(E, x) E dE &= \frac{1}{2\pi} \int_0^{E_0} dE E g(E) \varphi(E, x) \int e^{i(E'-E)t} dt = \\ &= \int_0^{E_0} g(E) \varphi(E, x) \delta(E' - E) E dE = g(E') E' \varphi(E', x); \end{aligned} \quad (113)$$

while its right part becomes

$$\begin{aligned} -\frac{1}{2\pi} \int dt e^{iE't} \int_0^{E_0} g(E) e^{-iEt} \frac{\partial^2 \varphi(E, x)}{\partial x^2} dE + \frac{1}{2\pi} \int dt e^{iE't} \int_0^{E_0} g(E) V(x, \bar{E}, t) e^{-iEt} \varphi(E, x) dE &= \\ = -\frac{1}{2\pi} \int_0^{E_0} dE g(E) \frac{\partial^2 \varphi(E, x)}{\partial x^2} \int e^{i(E'-E)t} dt + \frac{1}{2\pi} \int_0^{E_0} dE g(E) \varphi(E, x) \int V(x, \bar{E}, t) e^{i(E'-E)t} dt &= \\ = -g(E') \frac{\partial^2 \varphi(E', x)}{\partial x^2} + \frac{1}{2\pi} \int_0^{E_0} dE g(E) \varphi(E, x) \int V(x, \bar{E}, t) e^{i(E'-E)t} dt. \end{aligned} \quad (114)$$

As a result, we obtain eq. (112) in the form

$$g(E') E' \varphi(E', x) = -g(E') \frac{\partial^2 \varphi(E', x)}{\partial x^2} + \frac{1}{2\pi} \int_0^{E_0} dE g(E) \varphi(E, x) \int V(x, \bar{E}, t) e^{i(E'-E)t} dt. \quad (115)$$

## 9.2 The case of the simple Albreht's potential

Just as an example of a possible potential  $V(x, t)$ , let us choose

$$V(x, t) = V_0(x) + \gamma W_A(x). \quad (116)$$

where  $W_A(x)$  is the simple Albreht's dissipation term. Here,  $\gamma$  is a constant,  $V_0(x)$  is the usual stationary component of  $V(x)$ , and the dissipative component of  $V(x)$  has the form

$$W_A(x) = \langle p \rangle (x - \langle x \rangle), \quad (117)$$

where the averages are fulfilled by integrating over  $x$  by means of the functions  $\Psi^*(x, t)$  and  $\Psi(x, t)$ . For the right part of eq. (117) one gets

$$\begin{aligned} \langle p \rangle &= -i \int dx \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 g(E_1) g(E_2) e^{i(E_1-E_2)t} \varphi^*(E_1, x) \frac{\partial \varphi(E_2, x)}{\partial x}, \\ \langle x \rangle &= \int dx \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 g(E_3) g(E_4) e^{i(E_3-E_4)t} x \varphi^*(E_3, x) \varphi(E_4, x); \end{aligned} \quad (118)$$

so that the total potential  $V(x, t)$  becomes

$$\begin{aligned} V(x, t) &= V_0(x) - i\gamma \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 g(E_1) g(E_2) g(E_3) g(E_4) \\ &\times e^{i(E_1-E_2+E_3-E_4)t} (x-x_2) \varphi^*(E_1, x_1) \frac{\partial \varphi(E_2, x_1)}{\partial x_1} \varphi^*(E_3, x_2) \varphi(E_4, x_2). \end{aligned} \quad (119)$$

Taking into account this, we find the second term, in the r.h.s. of eq. (115), to be:

$$\begin{aligned} &\frac{1}{2\pi} \int_0^{E_0} dE g(E) \varphi(E, x) \int V(x, \bar{E}, t) e^{i(E'-E)t} dt = \\ &= \int_0^{E_0} dE g(E) \varphi(E, x) V_0(x) \delta(E' - E) - \\ &- i\gamma \int_0^{E_0} dE g(E) \varphi(E, x) \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 g(E_1) g(E_2) g(E_3) g(E_4) \\ &\times (x-x_2) \varphi^*(E_1, x_1) \frac{\partial \varphi(E_2, x_1)}{\partial x_1} \varphi^*(E_3, x_2) \varphi(E_4, x_2) \delta(E' - E + E_1 - E_2 + E_3 - E_4) = \\ &= g(E') \varphi(E', x) V_0(x) - \\ &- i\gamma \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 g(E_1) g(E_2) g(E_3) g(E_4) g(E'') \\ &\times (x-x_2) \varphi^*(E_1, x_1) \frac{\partial \varphi(E_2, x_1)}{\partial x_1} \varphi^*(E_3, x_2) \varphi(E_4, x_2) \varphi(E'', x), \end{aligned} \quad (120)$$

where

$$E'' = E' + E_1 - E_2 + E_3 - E_4. \quad (121)$$

As a consequence, the whole eq. (115) gets transformed into

$$\begin{aligned} &g(E') E' \varphi(E', x) = -g(E') \frac{\partial^2 \varphi(E', x)}{\partial x^2} + g(E') \varphi(E', x) V_0(x) \\ &- i\gamma \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 g(E_1) g(E_2) g(E_3) g(E_4) g(E'') \\ &\times (x-x_2) \varphi^*(E_1, x_1) \frac{\partial \varphi(E_2, x_1)}{\partial x_1} \varphi^*(E_3, x_2) \varphi(E_4, x_2) \varphi(E'', x) \end{aligned}$$

or (with the change of variables  $E' \rightarrow E$ )

$$\begin{aligned}
 & \left( -\frac{\partial^2}{\partial x^2} + V_0(x) - E \right) \varphi(E, x) = \\
 & = i\gamma \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 \frac{g(E_1)g(E_2)g(E_3)g(E_4)g(E'')}{g(E)} \\
 & \quad \times (x - x_2) \varphi^*(E_1, x_1) \frac{\partial \varphi(E_2, x_1)}{\partial x_1} \varphi^*(E_3, x_2) \varphi(E_4, x_2) \varphi(E'', x).
 \end{aligned} \tag{122}$$

We have thus obtained for this case the time-independent Schrödinger equation, by taking however into account dissipation via the parameter  $\gamma$ . Of course, when  $\gamma$  tends to zero, one goes back to the stationary Schrödinger equation.

### 9.3 Method of the successive approximations

Assuming the coefficient  $\gamma$  to be small, one can find the unknown function  $\varphi(x)$  in the simplified form

$$\varphi(x) = \varphi_0(x) + \gamma \varphi_1(x), \tag{123}$$

where as function  $\varphi_0(x)$  it has been used the standard WF of the time-independent Schrödinger equation with potential  $V_0(x)$  and energy  $E_0$ :

$$\left( -\frac{\partial^2}{\partial x^2} + V_0(x) \right) \varphi_0(x) = E_0 \varphi_0(x). \tag{124}$$

Substituting solution (123) into eq. (124), we obtain a new equation containing all the powers  $n$  of  $\gamma$ , namely, the  $\gamma^n$ . Let us confine ourselves, however, to write down this equation with accuracy up to  $\gamma^1$  only:

$$\begin{aligned}
 & \left( -\frac{\partial^2}{\partial x^2} + V_0(x) - E \right) \left( \varphi_0(E, x) + \gamma \varphi_1(E, x) \right) = \\
 & = i\gamma \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 \frac{g(E_1)g(E_2)g(E_3)g(E_4)g(E'')}{g(E)} \\
 & \quad \times (x - x_2) \varphi_0^*(E_1, x_1) \frac{\partial \varphi_0(E_2, x_1)}{\partial x_1} \varphi_0^*(E_3, x_2) \varphi_0(E_4, x_2) \varphi_0(E'', x),
 \end{aligned} \tag{125}$$

where the unknown  $\varphi_1(x)$  does not appear any longer, of course, into the r.h.s. of this equation. Taking  $E = E_0$ , we can rewrite in eq. (125), separately, the various terms with different powers of  $\gamma$ . When limiting ourselves to  $n = 0, 1$ , we obtain

$$\begin{aligned}
 \gamma^0: & \quad \left( -\frac{\partial^2}{\partial x^2} + V_0(x) - E_0 \right) \varphi_0(E_0, x) = 0, \\
 \gamma^1: & \quad \left( -\frac{\partial^2}{\partial x^2} + V_0(x) - E_0 \right) \varphi_1(E_0, x) = \\
 & = i\gamma \int dx_1 \int dx_2 \int_0^{E_0} dE_1 \int_0^{E_0} dE_2 \int_0^{E_0} dE_3 \int_0^{E_0} dE_4 \frac{g(E_1)g(E_2)g(E_3)g(E_4)g(E'')}{g(E_0)} \\
 & \quad \times (x - x_2) \varphi_0^*(E_1, x_1) \frac{\partial \varphi_0(E_2, x_1)}{\partial x_1} \varphi_0^*(E_3, x_2) \varphi_0(E_4, x_2) \varphi_0(E'', x),
 \end{aligned} \tag{126}$$

where

$$E'' = E_0 + E_1 - E_2 + E_3 - E_4. \quad (127)$$

The first equation holds when dissipation is absent. The second equation determines the unknown function  $\varphi_1$  in terms of the given  $\varphi_0$ : It results to be an ordinary differential equation of the second order, that can be solved by the ordinary numerical methods.

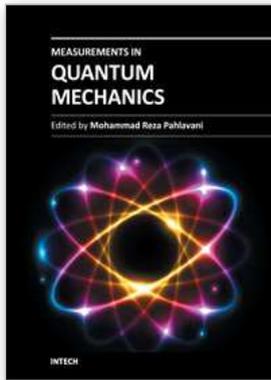
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Perhaps quantum mechanics is viewed as the most remarkable development in 20th century physics. Each successful theory is exclusively concerned about "results of measurement". Quantum mechanics point of view is completely different from classical physics in measurement, because in microscopic world of quantum mechanics, a direct measurement as classical form is impossible. Therefore, over the years of developments of quantum mechanics, always challenging part of quantum mechanics lies in measurements. This book has been written by an international invited group of authors and it is created to clarify different interpretation about measurement in quantum mechanics.

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### InTech Europe

University Campus STeP Ri  
Slavka Krautzeka 83/A  
51000 Rijeka, Croatia  
Phone: +385 (51) 770 447  
Fax: +385 (51) 686 166  
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### InTech China

Unit 405, Office Block, Hotel Equatorial Shanghai  
No.65, Yan An Road (West), Shanghai, 200040, China  
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元  
Phone: +86-21-62489820  
Fax: +86-21-62489821

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