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Rationalizing the Strength of Hydrogen-Bonded of Molybdate-Phosphonic acid Complex (1:2): Density Functional Theory Studies

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ABSTRACT

The relative stability of hydrogen-bonded of Molybdate-Phosphonic Acid (MPA) complex (1:2) in gas phase has been carried out using Density Functional Theory (DFT) methods. The methods are used for calculations are B3LYP, BP86 and B3PW91 that have been studied in two series of basis sets: D95** and 6-31+G(d,p) for hydrogen and oxygen atoms; LANL2DZ for Mo and Phosphorus. Predicted hydrogen-bond geometry and relative stability are discussed. Equilibrium geometry in the ground electronic state energy has been calculated for 1:2 complex. The best results for energetics and geometry of the ground state was obtained with BP86 calculations.

Keywords: Hyrogen bonding; Basis sets; Equilibrium structure.

INTRODUCTION

Among noncovalent interactions [1], hydrogen bonding [2] is of paramount significance.A vast vary supermolecular assemblies owe their well-defined structure to the existence of adjacent hydrogen-bond-donor and –acceptor units at complementary constituent parts [2,3]. The investigation of hydrogen bonding is also important for many practical applications, such as the design of antibiotics [4,5] and the development of new materials with programmed properties, e.g., ordered nanocomposites [5], photoresponsive sensors [5,6], and hydrogen-bonded networks resulting in thin films [7] or liquid crystals [8]. Recent investigations in polymer science have shown that π-conjugated oligomers functionalized with units capable of hydrogen bonding can form reversible polymers [3,9] and stacked hierarchic structures [10]. These aggregates can be used in electrooptical devices such as solar cell [11] and light-emitting diodes [12] with tunable macroscopic properties. The ability to understand and predict the stability of hydrogen-bonded systems is of importance for the rational development of these chemical technologies. A number of experimental and theoretical methods have been applied for analysis of the hydrogen-bonded systems [2] to obtain simple reliable models for interpreting their stabilities. Bader's "atoms in molecules" theory that describes any chemical bond by partitioning its electron density [13] has been very seminal in formulating several models allowing the linear [14,15] and nonlinear [16-20]

Correlations between electron density at the bond critical point and bond distance and thus the bond strength. The groups of Elguero [19,20] and Mó [21-23] as well as other authors [24] have shown the usefulness of the latter models in interpreting the strength of some simple hydrogen-bonded systems such as methanol-water, phosphonic acid, and phosphinoxides and aminoxides. Another model that distinguishes electrostatic interactions as a tool to predict hydrogen-bonding energies of complexes having more than one hydrogen bond in solution has been evolved on the basis on the Monte Carlo solution simulations by Jorgensen [25] and experimental studies by Schneider [26]. This concept has been widely applied and recommended as a useful guideline for interpreting stabilities and for designing new hydrogen-bonded associates [3,27-31]. Despite the lack of precise definition of a hydrogen bond, the statement that it is essentially of electrostatic nature [32] has been questioned by recent studies of low-barrier hydrogen bonds in enzyme catalysis [33,34] and theoretical remarks on the somewhat covalent nature of hydrogen bonding [35].

In this paper we investigate the hypothesis of rationalizations of stabilities of hydrogen-bonded species and hydrogen-bonded building blocks by means of DFT methods. DFT calculations of hydrogen-bonded at the B3LYP, BP86 and B3PW91 methods with two

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series of basis sets: D95** and 6-31+G (d,p) for hydrogen and oxygen atoms; LANL2DZ for Mo and Phosphorus have been carried out. The question of the nature of a hydrogen bond is not addressed in the present work. Hydrogen bonding will be discussed in terms of observable properties such as geometry and interaction energy. Earlier ab initio studies of the structures and stabilities of hydrogen-bonded assemblies of nucleic acid basis carried out [36-43] and show that quantum chemical techniques could now be used to perform calculations on molecular systems of practical significance.

METHODS

All DFT calculations were carried out with the Gaussian 98 program [45]. Geometry optimizations in the gas phase for all components and complex were performed at the DFT level with B3LYP, BP86 and B3PW91 functionals and with two series of basis sets:

A. Dunning basis set plus polarized functions (D95**) for hydrogen and oxygen atoms; LANL2DZ for Molybdenum and Phosphor. The effective core potential of Wadt and Hay is also included for Mo and P.

B. Double-zeta valance basis set plus polarized and diffuse functions (6-31+G(d,p)) for hydrogen and oxygen atoms; LANL2DZ for Molybdenum and Phosphor. The effective core potential of Wadt and Hay is also included for Mo and P.

This level that makes use of Becke-Style density functional theory [45] with the various correlation functionals (LYP, P86 and PW91) [46]. The double-ζ basis set adds two sizes of orbitals functions on heavy atoms and hydrogens, respectively, as well as diffuse functions on both.

The standard A and B basis sets were used in all calculations. Pople et al. have shown that the absolute deviations for the bond lengths and angles are smaller than corresponding values obtained at such levels of theory as MP2/6-31G(d) and QCISD/6-31G(d) [47]. The earlier studies of hydrogen binding in nucleic acid bases indicate that the Becke-Style density functional theory yields reliable interaction energies that correspond to the MP2/6-31G(d,p) level data [37]. Therefore, the B3LYP, BP86 and B3PW91 methods were applied in the all of calculations reported in this paper. The interaction energies of the counterparts estimated as the energy difference between the complex and the isolated components and were corrected for the basis set superposition error (BSSE).

DFT level optimizations of three methods with A and B basis sets resulted in very close geometries in each series of basis sets and also values of interaction energies as those obtained are closed.

RESULTS

Theoretical data of the calculated hydrogen-bond geometries for structure of MPA complex (1:2) results is given in Table 1 and the equilibrium structure obtained in the BP86/(H,O):D95**+(Mo,P):LANL2DZ that has minimum energy is shown in Figure 1.

Clearly, all of structural parameters have been undertaken many variations but we considered those that importance in hydrogen-bonded complex. Table 1 indicates the hydrogen-bond parameters in the species calculated by the DFT methods for B3LYP/A & B and B3PW91/A & B are closer than the values obtained by the BP86/A & B and Figures 2 and 3 show these trends. Particularly, these differences for energetics of equilibrium geometry are very highlight for Methods/A. According to previous studies, HF-optimized structures show essentially bigger deviations in hydrogen-bond lengths [48]. Both various groups of basis sets of DFT techniques showed similar trends in reproducing the hydrogen-bond angles. The source of the different of hydrogen-bond geometries from experimental may be attributed to a combination of two factors. First, the calculated structures are somewhat simplified analogues of the real systems. Second, as shown by Bickelhaupt et al., [49] the molecular environment in the crystal cell may cause significant disagreement between theory and experiment regarding hydrogen-bond lengths. Also, Leszczynski et al. have shown that the better agreement with experimental data and their literature reports cited [48], the discussion relies mostly on the DFT results. The longest hydrogen bonds correspond to O…H bonds present in MPA complex (1:2), while small deviations of hydrogen-bond angles from 180° manifest themselves in this complex. Interestingly, MPA complex (1:2), which according to the calculations are strongly bound species among the hydrogen-bonded systems have also the shortest hydrogen bonds and almost straight hydrogen-bond angles. The shorter hydrogen bonds and the straight hydrogen-bond angles do not necessarily reflect stronger binding. On contrary, with significantly high calculated interaction energies, display two O...H hydrogen bonds and deviation from 180° in the corresponding O-H…O angles.

Table 1. Theoretical Data on Hydrogen-Bond Geometries (Å, Deg) in MPA Complex (1:2)

Method	**Basis Set**	**Bond Length**		**Angle**	**Bond Length**		**Angle**	**Bond Length**		**Angle**	**Bond Length**		**Angle**
		H11…O2	**H11-O8**	**O2-H11-O8**	**H19…O3**	**H19-O15**	**O3-H19-O15**	**H12…O4**	**H12-O10**	**O4-H12-O10**	**H18…O5**	**H18-O17**	**O5-H18-O17**
B3LYP	A[a]	1.490	1.039	176.5	1.490	1.040	176.4	1.500	1.020	176.2	1.490	1.040	176.3
B3LYP	B[b]	1.506	1.030	176.3	1.500	1.040	176.3	1.510	1.030	176.1	1.510	1.030	176.1
BP86	A	1.463	1.060	176.4	1.460	1.060	176.3	1.470	1.050	176.2	1.470	1.050	176.3
BP86	B	1.469	1.060	176.1	1.470	1.060	176.2	1.470	1.060	176.0	1.470	1.060	177.0
B3PW91	A	1.470	1.040	176.5	1.470	1.040	176.4	1.480	1.030	176.2	1.480	1.030	176.4
B3PW91	B	1.483	1.040	176.3	1.480	1.040	176.4	1.490	1.030	176.2	1.490	1.030	176.2

[a] **A :** (H,O):D95**+ (Mo,P):LANL2DZ [b] **B :** (H,O):6-31+G**+(Mo,P):LANL2DZ

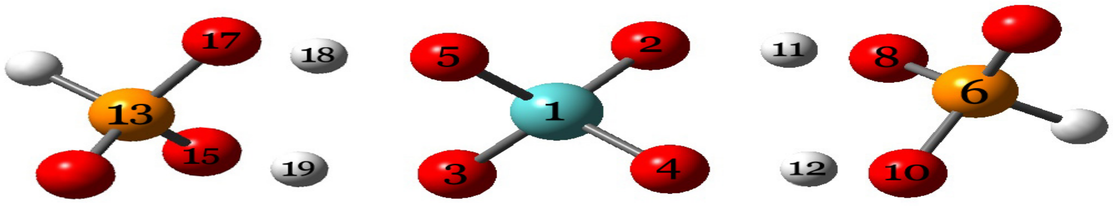

Fig.1. Equilibrium structure of MPA complex (1:2) in the P86/(H,O):D95**+(Mo,P):LANL2DZ.

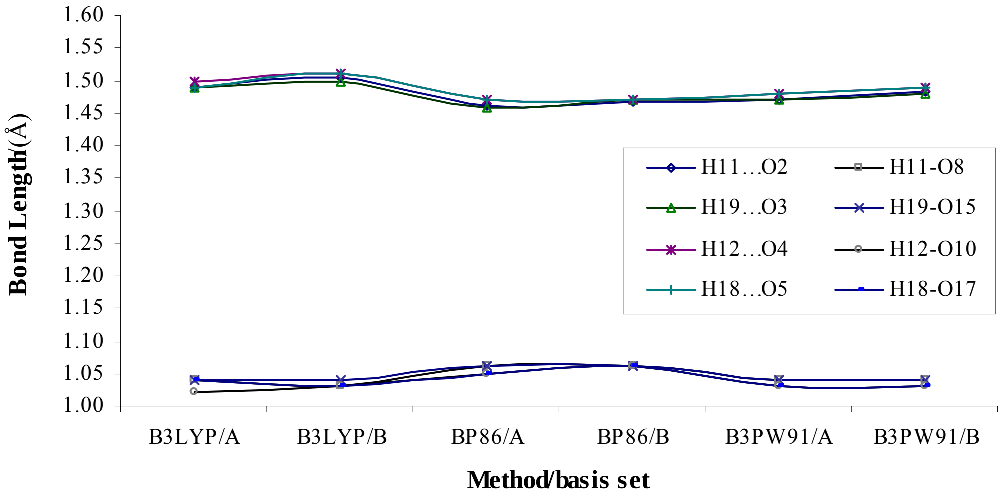

Fig. 2. Bond Lengths for MPA complex (1:2) for the indicated basis sets.

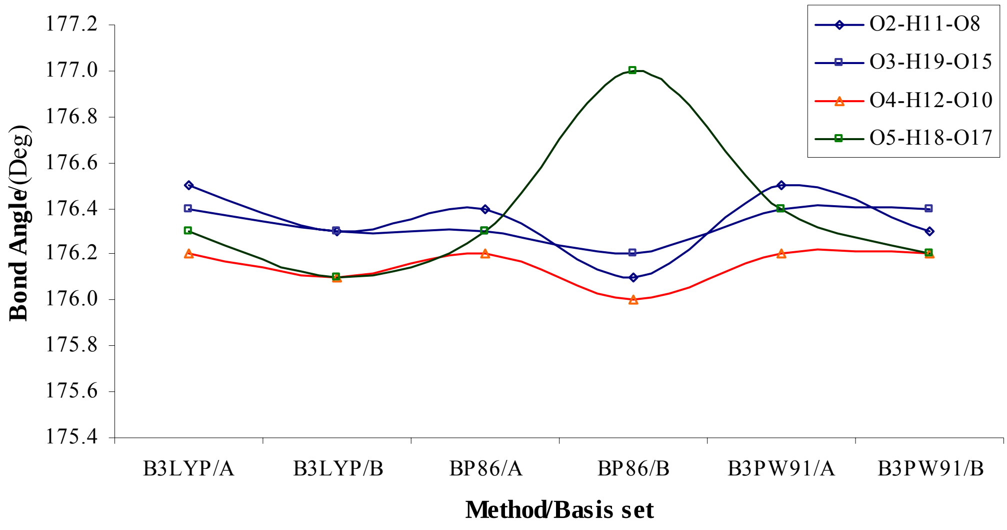

Fig.3. Bond Angles for MPA complex (1:2) for the indicated basis sets.

As mentioned in the Introduction section, there are several models evolved on the basis of Bader's theory showing linear or nonlinear relation between a bond length and electron density at the bond critical point. The latter value in turn reflects the strength of the bond. Therefore, the hydrogen-bond lengths can be used to some extent as indexes of the stabilization energy per hydrogen bond. Thus, the geometry analysis of hydrogen bonds in the calculated assemblies gives useful insights into internal cooperative effects regarding the complex stabilities but at the same time provides no general rules for any qualitative or semiquantitative conclusions concerning the relative stabilities of the complex (1:2). On the other hand the hydrogen-bond geometry data could be profitable for the critical evaluation of particular level of theory by the calculated molecular parameters [49]. Table 2 reports the calculated binding energies. The reported binding energies are with respect to computations at the three methods of density functional theory as mentioned in the Methods section, with A and B basis sets. Figure 4 shows these energies.

According to results that are shown in Table 2, the MPA complex (1:2) has minimum energy configuration with similar binding energies, differences between these energies that obtained by methods of DFT level as mentioned ratio to BP86/A are 2.8 (B3LYP/A) and 3.923 (B3PW91/A) kcal/mol and for BP86/B these differences are 2.041 (B3LYP /B) and 1.372 (B3PW91/B) kcal/mol, respectively.

Analogues of results that have been shown in Table 1, Table 2 indicates that the interaction energies that calculated by three methods for B3LYP/A & B and B3PW91/A & B are closer than the values obtained by the BP86/A & B. Also, in this investigation the configuration calculated of these DFT methods, with A basis set has shown more stability than the B basis set.

Table 2. Calculated Interaction Energies (kcal/mol) of The MPA Complex (1:2)

Method	Basis Set	Binding Energy
B3LYP	A[a]	-126.4
B3LYP	B[b]	-115.6
BP86	A	-129.2
BP86	B	-117.6
B3PW91	A	-125.3
B3PW91	B	-116.3

[a]**A :** (H,O):D95**+ (Mo,P):LANL2DZ
[b]**B :** (H,O):6-31+G**+(Mo,P):LANL2DZ

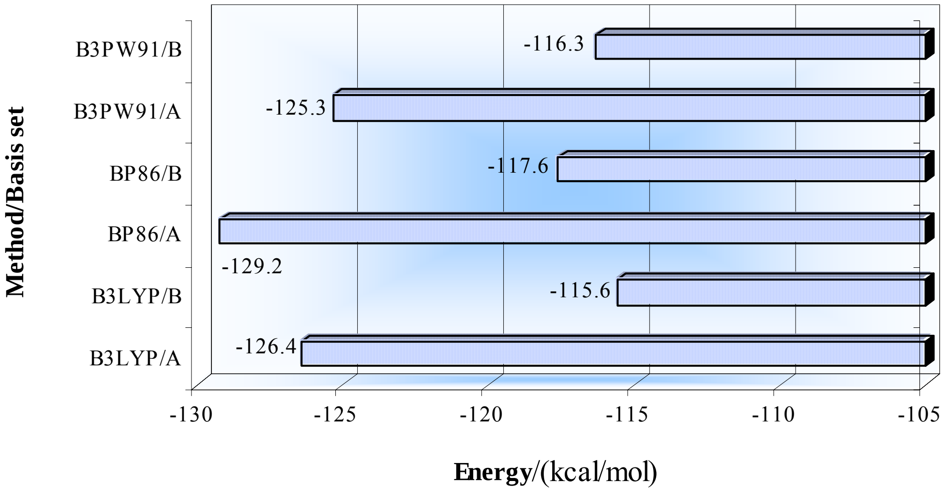

Fig. 4. Binding energies for MPA complex (1:2) for the indicated basis sets.

CONCLUSION

The results of our calculations indicate that the stability information of a complex (1:2) could not be directly used to obtain stability data for hydrogen-bonded assemblies in general. It is noteworthy that the geometry analysis of the hydrogen bonds can give useful insights into their cooperative effects affecting in this group of complex stabilities. Two conclusions are clear from this study: (1) the major difficulty with ab initio calculations of hydrogen-bonded interactions at the theory levels explored herein lies with inadequate basis set; and (2) systems with more than 3 or 4 heavy atoms (Mo, P, O, ...) are, at present, too expensive to treat accurately for both hardware and software reasons. The present study shows that the MPA complex (1:2) has minimum energy configuration with similar binding energies and the results obtained by the DFT methods for B3LYP/A & B and B3PW91/A & B are closer than the BP86/A & B. According to results of this paper, using DFT level for optimization of the geometry, the best results for energetics and geometry for this group of complex obtained by BP86/(H,O):D95**+(Mo,P):LANL2DZ calculations. Finally, we believe that the growing performance of ab initio methods may offer certain advantages in the rational design of new materials in the future.

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Path Integral Methods: Paths and Measurements

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ABSTRACT

In this paper, we explore the feasibility of a realistic interpretation of the quantum mechanical path integral that is, an interpretation according to which the particle actually follows the path that contribute to the integral. In this paper we have shown where all physical systems are in fact quantum, but in certain circumstances some of them may approximately be described as classical. This depends on the error with which the action of the system is known .

Keywords: Path integral; Continuous measurement, action; Feynman Paths; Probability, Amplitude Probability.

INTRODUCTION

The application of the Path Integral formalism to quantum continuous measurement and since has been analyzed in many different aspects. We now look at the problem from a wider point of view and formulate some perspectives in this direction. The aim of this paper is to show the peculiar role played by path in quantum physics . We shall see that, besides being an efficient mathematical formalism, paths form a powerful conceptual tool of quantum theory. As a result some paradoxical features of quantum mechanics become clearer or more consistent when formulated in terms of paths. [1, 2]

There questions will be considered in this connection: (1) the relation between quantum and classical, (2) the paradox of the two – slit experiment and (3) wave – particle dualism .

It –turns out that restricted path integrals provide a description of quantum processes which possesses both quantum and classical feature and allows a natural transition to its paradoxical features if it is analyzed in terms of “extended points”, i.e. point together with paths leading to them. Finally , the description of elementary particles in terms of paths allows one to take into account equally naturally both wave (global) and corpuscular (local) properties .

The latter point can be developed significantly in the framework of the relativistic theory on the basis of the group of paths. This provides an elegant and powerful group – theoretical basis for the most important areas of modern quantum field theory: gravity and gauge theory .

However, we conclude the phenomenon of wave function collapse (or state reduction) accompanying measurement will be discussed in the framework of the path – integral approach [3, 4]

The complex conceptual problems of quantum measurement theory will be mentioned in this connection .

QUANTUM AND CLASSICAL FEATURES IN CONTINUOUS MEASURMENT

In analyzing different situations time development of a quantum system with continuous measurement taken into account can be described by the measurement amplitude, or conditional (restricted) propagator

$$u_\alpha(q'', q' \ ) = \int_{q'}^{q''} d[q] \exp e\left(\frac{i}{h} s[q]\right) w_\alpha[q] \qquad (1)$$

Here α is the output of the measurement and   is a functional describing the restriction of path integration corresponding to information contained in this output [4, 5, and 6]

This equation is valid if a continuous measurement is performed in the time interval $[t', t'']$ then some information about this path is available, at least in principle.

This above information can be expressed by the (positive- valued)   functional w_α; Where

$$0 \le w_\alpha \le 1 \qquad (2)$$

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For the analysis one may understand α as the output of the coordinate monitoring (measurement of paths) of a particle or of some other system. Then can be identified with some path [a] (emerging as a result of measurement) and the functional w [q] is nonzero for path [q] close to [a]. Integration in equation (1) is then effectively limited by some corridor of paths around [a]. The width of the corridor a is nothing but an error of the coordinate monitoring. [7, 8]

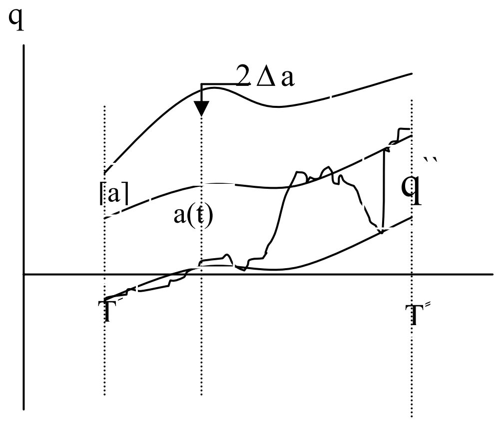


Fig.1. A corridor $\alpha = I_{[a]}$ describing the monitoring of coordinate (measurement of Position a path(

This verbal description of measurement can be made mathematically precise with the help of the inequality .

$$\left|q(t) - a(t)\right| \le \Delta a \qquad (3)$$

Then the result of the measurement

$$[a] = \{a(t) \ |t' \le t \le t''\}$$

Defines the set of path I[a] which can be described as a corridor of with 2Δa with the path [a] lying in the middle (fig 1) . the measurement amplitude U[a]in this case can be evaluated as a path integral [esq.(1)] over the corridor $a = I_{[a]}$. this procedure has been performed by Mensky (197 9) .[1, 2]

From the latter know that the evolution of the measured system can be described by the formula .

$$\left|\Psi'_\alpha\right> = U_\alpha \ \left|\Psi\right> \qquad (4)$$

Let us now analyze these formulas from the point of view if the relation between quantum and classical features of the system . The measurement output α is essentially classical because it arises as a result of the action of a classical measuring device. For example in the case if coordinate monitoring the output [a] is a trajectory of a particle (or a trajectory of a quantum system in its configuration space). In fact we have not just a single path [a] but a corridor of path around [a] However, This is not because a real particle is quantum but because real measurement has a finite precision (and there for finite error Δa). The restricted (conditional) propagator $U_{[\alpha]}$ is a typical quantum object, and operator acting on the wave function of a particle (or of some other system). Thus we have here both quantum and classical features of motion , and the description include both quantum and classical elements. The result of the evolution of the system may be described as its classical trajectory [a].

However, we know also that the wave function of the system, being originally $\left|\Psi\right>$, Becomes $\left|\Psi'_\alpha\right>$ after the measurement.

It was shown that in typical cases there are two radically different regime of measurement. Classical and quantum.

The classical regime arises if the measurement is rough enough ($\Delta\alpha << \Delta\alpha_{opt}$) and the quantum regime is characteristic of fine measurement ($\Delta\alpha << \Delta\alpha_{opt}$). Between these two regime of measurement ($\Delta_\alpha \approx \Delta\alpha_{opt}$) giving maximum information. Consider these regime from the point of view of the relation between the quantum and classical elements of the system's motion. The measurement output α can not be predicted unambiguously. There is always some variance in these outputs, $\delta\alpha$ in the classical regime of measurement ($\Delta\alpha >> \Delta\alpha_{opt}$) this variance coincides with the error of measurement. [9]

$$\delta\alpha = \Delta\alpha \qquad (5)$$

For example, the trajectory of a particle [a] obtained as a result of measurement in the classical regime coincides with the classical trajectory [q class] within the limits of the measurement error.Δα Thus the properties of the measurement results α are essentially classical in the classical in the classical regime of measurement [10] .

What can be said about the evolution of the wave function in the classical regime? it was emphasized latter that the restricted propagator U coincides in the classical regime of measurement with the unrestricted Feynman propagator U, i, e with the ordinary quantum – mechanical evolution operator thus in the classical regime the measurement result (for example the trajectory of a particle) is of a purely classical character, while the system wave function obeys a purely quantum evolution law (the Schrödinger equation). In the quantum regime of measurement ($\Delta\alpha << \Delta\alpha_{opt}$) the results of the measurement display of much wider variance than the error of measurement

$$\delta a = \frac{\Delta\alpha^2{}_{opt}}{\Delta\alpha} >> \Delta\alpha \qquad (6)$$

Thus purely classical characteristic of the motion (for example the trajectory of a particle) is strongly influenced by the quantum properties of the system. This may be called quantum measurement noise. In the case of position monitoring the measured trajectory [a] may deviate from the classical trajectory [q class] by much more than the measurement error,

$$\delta\alpha = \frac{\Delta a^2{}_{opt}}{\Delta a} >> \Delta a \qquad (7)$$

In the limit $\Delta a \to 0$ all path [a] have the some probability .

What can be said a bout the quantum element of description, the propagator u, in the quantum regime of measurement? The most interesting point is that instead of single unitary evolution operator u (as in the classical regime) we now have the set of partial evolution operator, Uα where α can be any measurement output from the set of probable outputs. [10, 11]

Instead of the conventional unitarily condition, the partial evolution operator must satisfy the generalized unitarily condition of the form

$$\sum_{\alpha} u^{+}_{\alpha} u_{\alpha} = 1 \qquad (8)$$

Nothing concrete can be said about each of the operator u_α in the general case of the quantum regime of measurement. Generally their behavior is rather complicated. It is easy, however, to consider the limit $\Delta a \to 0$ of the coordinate monitoring. In this case a very narrow corridor around some path [a] is obtained as a result of the measurement. One may say that in practice on path is found as a result of the measurements instead of a set of paths. According to this, just one path [a] (more precisely, a very narrow corridor around it) contributes to the path integral [eq.(1)]. The only action of the resulting propagator on the wave function (except for changing its norm) is then to change is phase by the value

$$\frac{s[a]}{\hbar} \quad \left|\Psi'_{[a]}\right> = e^{\frac{i}{\hbar}s[a]} \left|\Psi\right> \qquad (9)$$

THE TWO SLIT EXPERIMENT

This experiment is a classic illustration of the peculiarities of quantum mechanics; there is some paradoxical feature in this experiment. They are that the picture p12 appearing on the scintillation screen when both slits are open is not a simple sum of the picture, p1 and p2 seen when the first or second slit is open. This contradicts the classical view that the particle can reach some point x of the screen only through on of the slit (1 or 2), and thus the corresponding probabilities p1, p2 must be added to give the probability p12 of reaching the screen with both slit open. Of course this paradox arises only because the situation has been considered classically. We know the quantum procedure leading to the correct results, which consist in applying amplitudes instead of probabilities .

Form a certain point of view the main object in quantum mechanics is probability amplitude because it expresses the principle difference amplitude because it expresses the principle difference between quantum and classical theory. The probability amplitude of some event is a complex number A such that p= $|A|^2$ is the probability of this event. Quantum mechanics differs in that not probabilities but probability amplitudes should be summed up for a quantum system suppose that some event can occur through on of two alternative channels and that the probability amplitudes for these channels are A_1 and A_2. Then the complete probability amplitude for the event under consideration

$$A = A_1 + A_2 \qquad (10)$$

And its probability is

$$p = |A|^2 = |A_1 + A_2|^2 \qquad (11)$$

A typically example is a particle passing through one of two slits in an opaque screen (fig (2), with A_1 being the amplitude for the particle to pass through on of the slits and A_2 that for it to pass through the other. It is because of the law of amplitude summation (10) that passing through on of the slits can not be considered independently from passing through the other slit. The consequence of this law is an interference pattern at the scintillation screen when a series of particles passes through two slits the eq (10) is valid, however, only if there is no means of knowing which of two possible alternatives has actually occurred. In this case the alternatives are called, according to Feynman, interfering; they may also be called quantum alternatives. If an additional observation (measurement) is performed giving information about which route has been followed, then the amplitude summation rule change into the probability summation rule

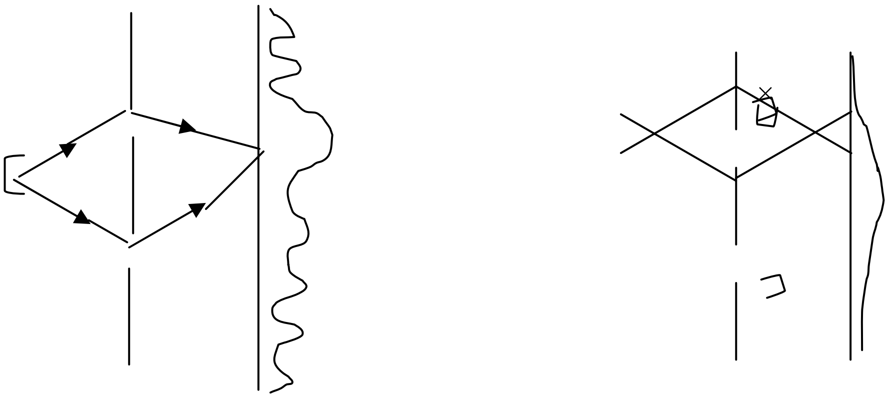
$$p = p_1 + p_2 = |A_1|^2 + |A_2|^2 \qquad (12)$$

As a consequence, no interference pattern will arise in the two- slit experiment if, for example, the flow of photon falls on the opaque screen so that scattering of the photons shows which of two slits the particle has passed through. In such a situation Feynman called the alternative incompatible .

It also seems convenient to use the term classical alternatives. The amplitude summation rule is also valid for many alternative channels .

$$A = A_1 + A_2 + \ldots\ldots + A_n \qquad (13)$$

Provided that there is no possibility of discovering which channel has been actually followed? If some observation (measurement) is performed giving information about the channel followed, then the amplitude summation rule must be corrected.



(a) (b)

Fig.2. the two-slit experiment lead to an interference pattern if it is not known which slit the particle has passes through.

The method of correction depends upon the information provided by the measurement. The information may be complete so that the channel followed is known precisely. Then the probabilities of separate channel should be summed instead of their amplitudes:

$$P=P_1+P_2+\ldots\ldots P_n \quad P_i=|A_i|^2 \qquad (14)$$

For another type of observation information may be only partial this means that the measurement is rougher. For example, let the measurement permit one to know whether the number of the channel followed belongs to one of the following pairs:

$$(1, 2) ;(3, 4) ;\ldots\ldots.(n-1, n) \qquad (15)$$

(We suppose that the total number of channel is even.)

(a) But it gives no interference if an additional observation shows which slit was used. **(b)** Then the probabilities corresponding to separate pairs are to be summed but amplitudes should summed inside the pairs

$$P=P_1+P_2+\ldots\ldots p_{\frac{n}{2}} \qquad p_i=\left|A_{2i-1}+A_{2i}\right|^2$$

In this case the alternatives inside each pair are interfering (quantum), while those in different pairs are incompatible (classical) alternatives channels may be divided in to triplets:

$$p=p_1+p_2+\ldots\ldots p_{n/3} \qquad p_i=\left|A_{2i-2}+A_{3i-1}\_A_{3i}\right|^2$$

Here P_i are probabilities for different results (out put) of measurement. For example, the value

$$p_i=\left|A_{2i-1}+A_{2i}\right|^2$$

In equation (14) is the probability for the ith pair to emerge as the output of the measurement. The value.

$$A_{\text{ith pair}}=A_{2i-1}+A_{2i} \qquad \mathbf{(16)}$$

Is nothing but the probability amplitude for the measurement to give the result expressed by the ith pair? More precisely this is the amplitude for the event under consideration to occur and the measurement of pairs of channels to show the ith pair the situation described by formulae (14) and (15) can be modeled in a many- slit experiment. The photon flow should then be directed at the opaque screen in such a way that pairs or triplets of slits could be distinguished by the photon scattering rather than individual slits .

However, we shall try to avoid the paradox in another way. Look for the origin of the paradox. It is that we have just one point x but different paths for reaching it [12, 13]

Evidently there would be no reason to try to add the probabilities if we were to consider different points in the situations denoted as 1, 2 and 12. The paradox could not arise in this case let us therefore try a new approach. Let us talk not about points on the screen but about extended points. Each extended point consists of point itself and all possible paths leading to it. Then in three versions of the two-slit experiment we have one ordinary point x but three different extended points x1, x_2 and x_{12}. The extended point x1 consists of the point x with the paths leading to this point through the first slit .

The extended point x_2 consists of the same point x but with the paths that lead to it through the same point x but with the paths that lead to it through the second slit. Finally the extended point x_{12} consists of the point x with the paths leading to it through both slit. Then there is no reason why the probabilities corresponding to the first two extended points should be added to give that corresponding to the third. This solution of the paradox seems at first glance to be unnatural because its essence is almost tautological: it boils down to a different way of saying the same thing; however, this renaming corresponds in our opinion to the spirit of quantum mechanics. The main idea in this renaming is that the target of the quantum process can not be considered separately from the process itself. The target (the point on the screen) has to be considered together with the process leading to it (the paths leading to this point). Only this combination (summarized in the image of an extended point), forms an adequate language for analyzing the phenomena is question. The same idea can be formulated in another way: it is more natural in quantum mechanics to deal with processes instead of state. Of course, normal practice is to consider states. However, there to be a tendency to more to the language of processes instead of the language of states. One argument in support of this is that any state is formed as a result of some process or other. It seems that the concept of an extended point accepted above is not a transition to processes instead of states but to considering processes (paths) together with states (Points). However, in accordance with the proceeding paragraph, the target point x can of course be represented adequately by paths leading to it. Therefore we way understand the extended point x_1,x_2,x_{12} as the corresponding sets of paths(leading to the point x through respectively slit 1, slit2 or both slits). The reader may see already that this final image is close to the sets of paths an introduced in this paper for analyzing continuous measurements. the advantage of the language of paths as a tool for solving the two-slit paradox is more evident if one take . In to consideration a possibility such as the delayed choice considered by miller and wheeler (1984). The point is that the two-slit experiment can be modified in a special way in this modification two different arrangement of the experiment are possible. In one the slit used by the particle is know after the experiment is over. In the other it is impossible to know this. It is only much later than the instant at which a particle enters a slit that the decision is made about whether the measurement should be performed according to one scheme or the other. Quantum interference effects arise only in the case when the slit used is not known .A delayed choice allows one to choose between interfering and none interfering schemes at the very last moment. [14, 15, and 16]

It is evident in this case that the whole history of a particle on its way to target paint is important for analysis of phenomenon. Thus only on extended point, the target together with the set of histories, is suitable for analysis. The general conclusion that can be drawn from this argument is that the language of paths is preferable to the language of points in quantum theory. There are two different (ways of using paths in quantum theory). One, discussed in detail in paper Feynman in year 1948 where called Feynman path integral approach. The other is the formalism of path- dependent wave function (or field) proposed by Mandelstam. (1962)

PATH AND CONTINUOUS MEASURMENTS

This argument may be applied to Feynman paths considered as quantum alternatives. The amplitude A (q'', q') for a particle to move from the point q' to the point q'' is called a propagator .

It has been expressed by Feynman (1948) in the form of sum (or rather integral) of the amplitudes A[q] corresponding to all possible paths [q] connecting the point q' and q''

$$A(q'',q') = \int A[q]d[q] \qquad (17)$$

Actually this formula is valid a propagator of any quantum system if q is understood as a coordinate (or a set of coordinates) of the configuration space of this system. For most arguments it is sufficient to consider a one- dimensional system. Formula (17) is analogous to equation (13) but for paths in the role of quantum alternatives. And analogously to the above argument equation (17) for the propagator is valid only if there is no possibility of finding out which path is followed when a particle move from q' to q''.

This is usually the case. However, suppose that a continuous measurement is performed simultaneously with this transition. Let the output α of this measurement give some information about the path of transition such information can be expressed by some set of paths I_α .If measurement give the result (out put) α then the transition follows on of the paths [q] belonging to the set I_α . Then, in analogy with equation (17), the amplitude for the transition from q' to q'' can be expressed as an integral over paths belonging to I_α :

$$A_\alpha(q'',q') = \int_{I_\alpha} A[q]d[q] \qquad (18)$$

The idea of using restricted path integrals in such a way was proposed in a short remark by Feynman (1948).A typical example of continuous measurement is monitoring of the coordinates of the system under consideration. Then the measurement gives the value a (t) of coordinate q (t) at each instant t (of some time interval) with the error Δa determined by the precision of measurement. α Then the output of measurement α can be identified with the path [a] expressed by the curve a (t). Knowing the output $\alpha = [a]$ of the position monitoring, one knows in fact that the actual path of the system [q] could differ from [a] by no more than the value Δa .

Therefore any path [q] lying in the corridor I_α of width $2\Delta a$ around [a] is possible, while no other path is impossible as an actual path of the system (taking the measurement output into α account). Information supplied by the measurement output α is expressed in this case by the corridor I_α of paths. Integration in the Feynman path integral should therefore be performed only over paths in the corridor I_α . [8, 9, and 10]

Moreover, the corridor I_α may be identified with the output α of the measurement. In fact this corridor represents the output of position monitoring better than the path [a] because also contains information about the error of measurement .the formula (18) will in fact be the basis for all our consideration in this paper.[17,18]

If α is fixed, the amplitude $A_\alpha = A_\alpha(q'',q')$ can be considered as the propagator of a particle undergoing continuous measurement (with the given output). If q' and q'' are fixed, the same amplitude can be thought of as probability amplitude for the continuous measurement to give the result α. Taking a square modulus of the amplitude, one can obtain the probability density for different out puts of the continuous measurement. A more general class of quantum continuous measurement can be described by the formula .

$$A_\alpha(q'',q') = \int w_\alpha[q]A[q]dq \qquad (19)$$

Here integration is performed over all paths connecting the point q' and q'' ,but with the functional w_α expressing information contained in the output α of the measurement .In the light of this information on the system follows a path for which w_α is large. The smaller is w_α [q], the less probable is it that the path [q] is taken by the system .

Generalization of the formulas (18) and (19) to the case of an arbitrary quantum system and arbitrary continuous easement is straightforward. Generalization is also possible for the easement of the configuration of a quantum field. (In the latter case the measurement can be continual because it is not only prolonged in time but also protracted in space.)

WAVE- PARTICLE-DUALISM

The situation with two slits is one illustration of wave-particle dualism typical of quantum mechanics. The essence of this dualism is that there are two aspects of quantum objects, in which they resemble a wave or a particle in the classical sense. Neither of these aspects can be abandoned; there are situation in which each of them becomes important. The analysis of the two- slit experiment in section before suggest, that the language of sets of paths could clarify some feature of the wave-particles dualism .

Here we shall consider question in more detail. Let us take for our analysis the typical continuous measurement, the monitoring of position of (say) a particle. As has been argued in section 1, the result of such a measurement is represented by the trajectory [a]. Thus the particle obtains the typical corpuscular characteristic of position at a definite instant, a (t).

The precision of the measurement, or its error, Δ_a determines the precision with which this characteristic is known. This type of continuous measurement therefore gives us a picture of a particle, not a wave. However, we see as a result of the analysis (see section 1) that the measurement gives results not characteristic of classical theory. The measured trajectory [a] may differ from the classical trajectory [q class] of a particle by value much greater than the measurement error Δa. Thus our object, though described by the same mathematical tools as a particle (position, trajectory), is not a classical particle. We can judge about this when observing its motion. Moreover, to describe this object completely, its wave function, or the state vector, $|\Psi>$, is necessary. This presents the wave aspects of the object. When observing the particle-like behavior of the object (its measured trajectory[a]), we obtain results that depend on its wave characteristics before the observation (its initial state $|\Psi>$,). But the most complete picture of the interrelation between the corpuscular and wave properties of a quantum particle is expressed by the restricted (conditional or spatial) propagator U[a]. In fact the discussion in section (1) of the interrelation between the quantum and classical properties of a particle is nothing but a representation (in different term) of its wave-particle dualism the partial propagator U[a] (and therefore the evolution of a quantum particle) has both quantum and classical (wave and corpuscular) features. As a propagator (evolution operator), it is quantum and describes the propagation of a wave. However, this quantum evolution only in the framework of a definite classical alternatives [a] .Each of these alternatives is described by classical (corpuscular) term(a trajectory) and their statistics is purely classical (probabilities but not amplitude).one may say that the path- integral theory of continuous measurements presents a corpuscular picture of a particle's motion along a trajectory , but in each actual evolution , for a given trajectory , quantum evolution acts: the wave propagates in a tube(corridor) corresponding to the trajectory . We see thus that the wave- particle dualism of quantum objects may be adequately represented with the help of the formalism of restricted path integrals. However, there is another application of path in quantum theory that also has something to do with wave-particle dualism-we mean the formalism of wave functions depending on paths instead of points. The arguments of section 2 show that path-dependent functions way are of some help even in no relativistic quantum mechanics. Such functions were introduced by Mandelstam (1962) in the framework of quantum electrodynamics and generalized to the case of non-Aeolian gauge field by Bialynicki-Birula (1963).the goal was the construction of an explicitly gauge-invariant formalism. [19, 20, 21]

CONCPTUAL PROBLEMS

The starting point for the discussion in this paper is the Feynman path integral. Restriction of the region of integration has been shown to describe the influence of the measuring device on the quantum system subject to continuous measurement such an influence is usually referred to as reduction of the system state or collapse of its wave function . In our case we mean continuous reduction corresponding to continuous measurement. However , the general conceptual problems that usually arise in connection with state reduction are shared by this type of measurement too. Let us discuss them briefly.

1. Continuous state reduction

In conventional quantum measurement theory state reduction is taken into account by the special procedure of von Neumann's projection or some generalization of it, instead of this, in the present approach the continuous state reduction resulting from continuous measurement is taken into account automatically by restriction of the path integral. This is one of the most important advantages of the path integral approach: the same procedure of integral restriction gives both the probability distribution of the measurement output and the reduction of the state under the influence of this measurement of course one should keep in mind that this type of continuous reduction (like any other) is an idealization. The influence of a real measurement device may differ from this idealized influence. The restriction of the path integral suggests implicitly that the influence of the measurement is in some sense the minimal influence necessary to obtained it the given type of information. The same information can be obtained from a poorer device that has a stronger influence on the system. [21, 22, and 23]

However, it is impossible to obtain the same information with a smaller influence. This is why the path- integral results in absolute quantum restriction on measurability . No device providing the required information (specified by the functional w_α) can have less influence than is described by restriction of the path integral. There is a class of measuring devices with just this minimum influence on the system supplying the required information (the theory says nothing about how these devices may by constructed) . All other devices work less efficiently ,providing less measurability than is found from the path integral approach. In fact, even the latter non-ideal case may be treated in the framework of the path-integral method . Indeed , if the device is non-ideal (for the given type of measurement), it is because it gives additional information about the system under investigation . Therefore this device non-ideal in the sense of the given type of measurement , is ideal for measurement of a different type, giving more information. Such a measuring device and its influence may also be described by restriction of the path . Integral, but with restriction to narrow sets of paths. Of course, the choice of the system of functional w_α restricting the path integral for the given system undergoing the given measurement is in practice a complicated task [4, 8, and 24].

2. What is collapse?

The remark made in section 1 is a technical one. It claims now state reduction (wave function collapse) is taken into account in the present approach. There is, however, an important and not quite clear conceptual question: what is collapse a how does it occur? The problem is that a description of collapse (like a description of any other aspect of measurement) necessarily includes classical elements . If one thinks (as many people do) that a quantum-mechanical description of any system is completely correct while the classical description is approximate , then the emergence of classical elements in the formalism of quantum measurement should have a purely quantum mechanical explanation. For this aim one may (and in fact must) include the measuring device in the consideration explicitly. This device should be described as an ordinary quantum system. Interacting in some way or other with the measured system. One may hope to obtain , in the framework of an ordinary quantum – mechanical analysis of these systems, the same result as in the quantum- measurement analysis including collapse of the wave function . This approach , however, faces major difficulties because different states of the measuring device arise in quantum superposition instead of a mixture. The difference between these two situations in similar to the difference between quantum(interfering) and classical (incompatible) alternatives . the phenomenon of decoherentization consisting in the loss of information about phases between alternatives states cannot be described in the frame work of unitary quantum-mechanical evolution and requires something like state reduction . One can formulate this difficulty as follows: if the measurement device is considered as a quantum system , then the question arises of how the state of this system can be identified. In other words, the measuring device should also be measured , and instead of solving the problem we only move it elsewhere . The real problem in this context is the investigation of decoherentization as a specific process, connecting essentially quantum (us observable in principle) and essentially classical (observable with negligibly small back influence) systems or states. Decoherntization may be introduced into the description of the quantum system under investigation or into the description of the measuring device but in both cases this stage is typical of the quantum theory of measurements but is not part of conventional quantum mechanics. There have been many attempts to avoid this peculiar stage of decoherentization. One of the exotic is the Everett-wheeler many-worlds interpretation of quantum mechanics(see ref(23)) in which the suggestion is accepted that different alternatives (different outputs of measurement) are all realized but in different worlds, and only one of these worlds is available for our observation. This explanation, though very interesting, does not seem quite satisfactory because instead of actually solving the problem it just converts one problem in to another. In any case, the existence of different world poses at least as many questions as it solves. There is a more convincing direction in which to search for a solution. Some investigators have tried to derive the picture of decoherentization as an approximate description of a quantum measuring device. The approximation is usually justified by a characteristic feature of the device, namely that it has vast number of degree of freedom and possesses instability of a definite type. Most experts now accept the picture of zurek (1981) According to this the interaction with the measuring device results in correlation between the states of the system and the states of the device while the interaction with the environment supplied a sort of discussion converting the superposition of these correlated states in to a mixture of them (the decoherentization process).the approach considered in this paper is purely phenomenological. It presents effective tools for describing collapse arising in the course of complicated (continuous and continual) measurement, but it does not describe the mechanism of the collapse. More over, no explicit model of the measuring device or environment is needed for the present approach . The advantage of this is a universal (model-independent) character of the conclusions drawn from the present approach. One possible miss understanding should be avoided in this connection. Some people think that no problem of collapse exist at all because real measurement can be described completely and correctly in the framework of ordinary quantum mechanics (without elements characteristic of the quantum theory of measurement, such as collapse) if one take into account both the measured and the measuring systems. One may think then that there is no need for a quantum theory of measurement. In a sense, there is in deeded no need.

Any particular system in any regime of measurement can be considered in the framework of conventional quantum mechanics without using the methods of the quantum theory of measurement.

However, the quantum theory of measurement allows one to consider situations in great generality and reach some general conclusions which hardly be achieved by analyzing particular situations. Moreover, some problem of a general character can not even be formulated without the tools of the quantum theory of measurement consideration of the motion of photons in Heisenberg's δ -microscope leads to the same conclusions as the uncertainty principle, but the latter is very important because of its generality as an effective instrument of physical analysis[23,24,25,26].

The final conclusion from this analysis is that the problem of collapse can be avoided in practical calculations but inevitably emerges on the theoretical (conceptual) level. however ,even in practical investigations the quantum theory of measurement with its picture of wave function collapse is useful (in fact necessary) firstly for simplifying computations and secondly for obtaining general results of the type of the uncertainty principle obtaining general conclusion of this type is one of the goals of modern quantum measurement theory[27]. The hypothesis is sometimes put forward that the consciousness of an observer plays an important role in the phenomenon of state reduction (collapse). This idea began with the founders of quantum mechanics of modern paper let us mention an interesting one by squire (1988). The motivation for investigation in this direction is the apparent impossibility of solving the conceptual problem of collapse and the resulting conclusion that quantum-mechanics is not closed in itself .

3. Quantum-classical Evolution

In one way another, measurements lead to the emergence of classical elements in the description of a quantum system. In the path-integral approach this is seen in modification of the evolution law (see section 1). With the measurement taken into account evolution described by the set of (alternative) operators u_α where α the measurement output is. The purely classical element α arises in this description as a sign of influence of the measuring device. This may be treated in a wider manner as the influence of some sort of measuring medium. In fact a new type of evolution law is introduced in the framework of the present approach. The question then arises (connected with tae discussion of section 2) of what is the status of this quantum-classical evaluation law. It is evident that some sort of measurement is always performed in a real situation. Indeed, measurement in our sense is nothing other than obtaining information about the state of the system and putting it in classical forms so that it can be read without further disturbance of the system.

However, such information is always present (for example a rough estimation of the position of an elementary particle). One may say that any quantum system moves in a measuring medium of some sort or other . On the other hand, the influence of this medium in some particular situation may be negligible so that the ordinary quantum-mechanical evolution law is valid. This situation was analyzed in section (1). It is important that the boundary between the quantum system and the measuring device (medium) can be introduced in different place. Let us imagine for simplicity that there is a chain of systems.so,s1,s2,…. Each measuring the preceding one. Then one may consider just one system so explicitly , taking all the other in to account by restricting the path integral of the system so. The influence of the measurement (expressed by the restriction on the path integral) will then be comparatively large. Instead of this one can treat the (interacting) systems s0,s1explicitly, and take all the others into account by restricting the path integral of this compound system. Then the influence of measurement may be less. Finally one may consider explicitly sufficiently many subsystems so that the influence of all other is negligible. Then the purely quantum-mechanical description becomes correct. This is a specific formulation of a general argument in section 2. It may be said therefore that the description of a real system in the framework of the path-integral theory of continuous measurement is an approximation to reality. An opposite and intriguing point of view is also possible [14,28], namely that continuous reduction is a necessary counter part in the description of quantum systems. This means that collapse is supposed to occur spontaneously, without any special device or medium to cause it. The theory of quantum system in this case should differ from conventional quantum mechanics, including some features of quantum measurement theory as its internal features. For example, one may think that the restriction of path integrals is a necessary part of the right theory let us note in conclusion that the restriction of path integrals allows one to naturally overcome purely mathematical difficulties in their definitions [29]. Indeed , the restriction of a no relativistic path integral to a corridor (even one arbitrary wide) in coordinates and velocities make this integral a mathematically well defined object, unlike the original Feynman path integral. If a restriction in velocity turns out to be sufficient, a restriction of this type can be readily justified as describing a real physical situation when it is known in advance that the coordinates and their derivatives can not be arbitrary large[30]

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