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Quantum-like representation algorithm for probabilsitic data

We present a quantum-like representation algorithm, QLRA, for probabilistic data obtained in any domain of science. Quantum-like (QL) information representation is considered as incomplete information representation. This approach is applied to QL-simulation of processing of information by cognitive systems.

1. Introduction

We discuss the possibility to represent statistical data in the quantum-like (QL) way – by complex probability amplitudes, cf. [1]–[3]. Such a QL-representation provides the possibility to process data in complex Hilbert space and, hence, to use the standard description of quantum information theory. We present quantum-like representation algorithm (QLRA), which can be applied to statistical data obtained in any domain – cognitive and social sciences, psychology, economy and even political sceince. In our model QL-randomness appears not as irreducible randomness, but as a consequence of obtaining or/and using incomplete information about a system. We prefer to escape a rather heavy discussion on completeness of quantum physics, see [4]–[10], cf. [11], [12]. It might be that the real physical quantum randomness is really irreducible. Nevertheless, even in this case one might proceed in other domains of science by using QLRA and hence by interpreting QL information as incomplete information about a system. In this paper we consider in a more detail one special application – QL modeling of brain's functioning. The brain is modeled as a QL-computer.

We present a contextualist statistical realistic model for quantum-like representations in cognitive science and psychology [13], [14]. We apply this model to describe cognitive experiments to check quantum-like structures of mental processes. The crucial role is played by the *interference of probabilities for mental observables.* Recently one such experiment based on recognition of images was performed, see [13], [15]. This experiment confirmed our prediction on the quantum-like behavior of mind. In our approach "quantumness of mind" has no direct relation to the fact that the brain (as any physical body) is composed of quantum particles. We invented a new terminology "quantum-like (QL) mind." Cognitive QL-behavior is characterized by a nonzero *coefficient of interference* λ ("coefficient of supplementarity"). This coefficient can be found on the basis of statistical data. There are predicted not

only $\cos\theta$-interference of probabilities, but also hyperbolic $\cosh\theta$-interference. The latter interference was never observed for physical systems, but we could not exclude this possibility for cognitive systems. We propose a model of brain functioning as a QL-computer. We shall discuss the difference between quantum and QL-computers.

From the very beginning we emphasize that our approach has nothing to do with *quantum reductionism,* cf. [17]–[20]. Of course, we do not claim that our approach implies that quantum physical reduction of mind is totally impossible. But our approach could explain the main QL-feature of mind — *interference of minds* — without reduction of mental processes to quantum physical processes. Regarding the quantum logic approach we can say that our contextual statistical model is close mathematically to some models of quantum logic [16], but interpretations of mathematical formalisms are quite different. The crucial point is that in our probabilistic model it is possible to combine *realism* with the main distinguishing features of quantum probabilistic formalism such as *interference of probabilities, Born's rule, complex probabilistic amplitudes, Hilbert state space, and representation of (realistic) observables by operators.*

2. Observational Contextual Statistical Model

A general statistical realistic model for observables based on the contextual viewpoint to probability will be presented. It will be shown that classical as well as quantum probabilistic models can be obtained as particular cases of our general contextual model, the *Växjö model.*

This model is not reduced to the conventional, classical and quantum models. In particular, it contains a new statistical model: a model with hyperbolic *cosh*-interference that induces "hyperbolic quantum mechanics" [13].

A physical, biological, social, mental, genetic, economic, or financial *context C* is a complex of corresponding conditions. Contexts are fundamental elements of any contextual statistical model. Thus construction of any model M should be started with fixing the collection of contexts of this model. Denote the collection of contexts by the symbol $\mathcal{C}$ (so the family of contexts $\mathcal{C}$ is determined by the model M under consideration). In the mathematical formalism $\mathcal{C}$ is an abstract set (of "labels" of contexts).

We remark that in some models it is possible to construct a set-theoretic representation of contexts – as some family of subsets of a set Ω. For example, Ω can be the set of all possible parameters (e.g., physical, or mental, or economic) of the model. However, in general we *do not assume the possibility to construct a set-theoretic representation of contexts.*

Another fundamental element of any contextual statistical model M is a set of observables $\mathcal{O}$: each observable $a \in \mathcal{O}$ can be measured under each complex of conditions $C \in \mathcal{C}$. For an observable $a \in \mathcal{O}$, we denote the set of its possible values ("spectrum") by the symbol X_a.

We do not assume that all these observables can be measured simultaneously. To simplify considerations, we shall consider only discrete observables and, moreover, all concrete investigations will be performed for *dichotomous observables.*

Axiom 1: *For any observable $a \in \mathcal{O}$ and its value $x \in X_a$, there are defined contexts, say C_x, corresponding to x-selections: if we perform a measurement of the observable a under the complex of physical conditions C_x, then we obtain the value $a = x$ with probability 1. We assume that the set of contexts $\mathcal{C}$ contains C_x-selection contexts for all observables $a \in \mathcal{O}$ and $x \in X_a$.*

For example, let a be the observable corresponding to some question: $a = +$ (the answer "yes") and $a = -$ (the answer "no"). Then the C_+-selection context is the selection of those participants of the experiment who answering "yes" to this question; in the same way we define the C_--selection context. By Axiom 1 these contexts are well defined. We point out that in principle a participant of this experiment might not want to reply at all to this question. By Axiom 1 such a possibility is excluded. By the same axiom both C_+ and C_--contexts belong to the system of contexts under consideration.

Axiom 2: *There are defined contextual (conditional) probabilities $\mathbf{P}(a = x|C)$ for any context $C \in \mathcal{C}$ and any observable $a \in O$.*

Thus, for any context $C \in \mathcal{C}$ and any observable $a \in O$, there is defined the probability to observe the fixed value $a = x$ under the complex of conditions C.

Especially important role will be played by probabilities:

$$p^{a|b}(x|y) \equiv \mathbf{P}(a = x|C_y), a, b \in \mathcal{O}, x \in X_a, y \in X_b,$$

where C_y is the $[b = y]$-selection context. By axiom 2 for any context $C \in \mathcal{C}$, there is defined the set of probabilities:

$$\{\mathbf{P}(a = x|C) : a \in \mathcal{O}\}.$$

We complete this probabilistic data for the context C by contextual probabilities with respect to the contexts C_y corresponding to the selections $[b = y]$ for all observables $b \in \mathcal{O}$. The corresponding collection of data $D(\mathcal{O}, C)$ consists of contextual probabilities:

$$\mathbf{P}(a = x|C), \mathbf{P}(b = y|C), \mathbf{P}(a = x|C_y), \mathbf{P}(b = y|C_x), ...,$$

where $a, b, ... \in \mathcal{O}$. Finally, we denote the family of probabilistic data $D(\mathcal{O}, C)$ for all contexts $C \in \mathcal{C}$ by the symbol $\mathcal{D}(\mathcal{O}, \mathcal{C})(\equiv \cup_{C \in \mathcal{C}} D(\mathcal{O}, C))$.

Definition 1. (Växjö Model) *An observational contextual statistical model of reality is a triple*

$$M = (\mathcal{C}, \mathcal{O}, \mathcal{D}(\mathcal{O}, \mathcal{C})) \tag{2.1}$$

where $\mathcal{C}$ is a set of contexts and $\mathcal{O}$ is a set of observables which satisfy to axioms 1,2, and $\mathcal{D}(\mathcal{O}, \mathcal{C})$ is probabilistic data about contexts $\mathcal{C}$ obtained with the aid of observables belonging $\mathcal{O}$.

We call observables belonging the set $\mathcal{O} \equiv \mathcal{O}(M)$ *reference of observables.* Inside of a model M observables belonging to the set $\mathcal{O}$ give the only possible references about a context $C \in \mathcal{C}$.

3. Contextual Model and Ignorance of Information

Probabilities $\mathbf{P}(b = y|C)$ are interpreted as *contextual (conditional) probabilities.* We emphasize that we consider conditioning not with respect to *events* as it is typically done in classical probability [21], but conditioning with respect to contexts – complexes of (e.g., physical, biological, social, mental, genetic, economic, or financial) conditions. This is the crucial point.

On the set of all events one can always introduce the structure of the *Boolean algebra* (or more general σ-algebra). In particular, for any two events A and B their set-theoretic intersection $A \cap B$ is well defined and it determines a new event: the simultaneous occurrence of the events A and B.

In contract to such an event-conditioning picture, if one have two contexts, e.g., complexes of physical conditions C_1 and C_2 and if even it is possible to create the set-theoretic representation of contexts (as some collections of physical parameters), then, nevertheless, their set-theoretic intersection $C_1 \cap C_2$ (although it is well defined mathematically) need not correspond to any physically meaningful context. Physical contexts were taken just as examples. The same is valid for social, mental, economic, genetic and any other type of contexts.

Therefore even if for some model M we can describe contexts in the set-theoretic framework, there are no reasons to assume that the collection of all contexts $\mathcal{C}$ should form a σ-algebra (Boolean algebra). This is the main difference from the classical (noncontextual) probability theory [21].

One can consider the same problem from another perspective. Suppose that we have some set of parameters Ω (e.g., physical, or social, or mental). We also assume that contexts are represented by some subsets of Ω. We consider two levels of description. At the first level a lot of information is available. There is a large set of contexts, we can even assume that they form a σ-algebra of subsets $\mathcal{F}$. We call them the first level contexts. There is a large number of observables at the first level, say the set of all possible random variables $\xi : \Omega \to \mathbf{R}$ (here $\mathbf{R}$ is the real line). By introducing on $\mathcal{F}$ a probability measure $\mathbf{P}$ we obtain the classical Kolmogorov probability model $(\Omega, \mathcal{F}, \mathbf{P})$, see [21]. This is the end of the classical story about the probabilistic description of reality. Such a model is used e.g. in classical statistical physics.

We point our that any Kolmogorov probability model induces a Växjö model in such a way: a) contexts are given by all sets $C \in \mathcal{F}$ such that $\mathbf{P}(C) \neq 0$; b) the set of observables coincides with the set of all possible random variables; c) contextual probabilities are defined as Kolmogorovian conditional probabilities, i.e., by the Bayes formula: $\mathbf{P}(a = x|C) = \mathbf{P}(\omega \in C : a(\omega) = x)/\mathbf{P}(C)$. This is the Växjö model for the first level of description.

Consider now the second level of description. Here we can obtain a *non-Kolmogorovian Växjö model.* At this level only a part of information about the first level Kolmogorovian model $(\Omega, \mathcal{F}, \mathbf{P})$ can be obtained through a special family of observables $\mathcal{O}$ which correspond to a special subset of the set of all random variables of the Kolmogorov model $(\Omega, \mathcal{F}, \mathbf{P})$ at the first level of description. Roughly speaking not all contexts of the first level, $\mathcal{F}$ can be "visible" at the second level. There is

no sufficiently many observables "to see" all contexts of the first level – elements of the Kolmogorov σ-algebra $\mathcal{F}$. Thus we should cut off this σ-algebra $\mathcal{F}$ and obtain a smaller family, say $\mathcal{C}$, of visible contexts. Thus some Växjö models (those permitting a set-theoretic representation) can appear starting with the purely classical Kolmogorov probabilistic framework, as a consequence of ignorance of information. If not all information is available, so we cannot use the first level (classical) description, then we, nevertheless, can proceed with the second level contextual description.

We shall see that starting with some Växjö models we can obtain the quantum-like calculus of probabilities in the complex Hilbert space. Thus in the opposition to a rather common opinion, we can derive a *quantum-like description for ordinary macroscopic systems* as the results of using of an incomplete representation. This opens great possibilities in application of quantum-like models outside the micro-world. In particular, in cognitive science we need not consider composing of the brain from quantum particles to come to the quantum-like model.

Example 1. (Firefly in the box) Let us consider a box which is divided into four sub-boxes. These small boxes which are denoted by $\omega_1, \omega_2, \omega_3, \omega_4$ provides the the first level of description. We consider a Kolmogorov probability space: $\Omega = \{\omega_1, \omega_2, \omega_3, \omega_4\}$, the algebra of all finite subsets $\mathcal{F}$ of Ω and a probability measure determined by probabilities $\mathbf{P}(\omega_j) = p_j$, where $0 < p_j < 1, p_1 + ... + p_4 = 1$. We remark that in our interpretation it is more natural to consider elements of Ω as *elementary parameters,* and not as *elementary events* (as it was done by Kolmogorov).

We consider two different disjoint partitions of the set Ω :
$$A_1 = \{\omega_1, \omega_2\}, A_2 = \{\omega_3, \omega_4\},$$
$$B_1 = \{\omega_1, \omega_4\}, B_1 = \{\omega_2, \omega_3\}.$$

We can obtain such partitions by dividing the box: a) into two equal parts by the vertical line: the left-hand part gives A_1 and the right-hand part A_2; b) into two equal parts by the horizontal line: the top part gives B_1 and the bottom part B_2.

We introduce two random variables corresponding to these partitions: $\xi_a(\omega) = x_i$, if $\omega \in A_i$ and $\xi_b(\omega) = y_i \in$ if $\omega \in B_i$. Suppose now that we are able to measure only these two variables, denote the corresponding observables by the symbols a and b. We project the Kolmogorov model under consideration to a non-Kolmogorovian Växjö model by using the observables a and b – the second level of description. At this level the set of observables $\mathcal{O} = \{a, b\}$ and the natural set of contexts $\mathcal{C}$: $\Omega, A_1, A_2, B_1, B_2, C_1 = \{\omega_1, \omega_3\}, C_1 = \{\omega_2, \omega_4\}$ and all unions of these sets. Here "natural" has the meaning permitting a quantum-like representation (see further considerations). Roughly speaking contexts of the second level of description should be large enough to "be visible" with the aid of observables a and b.

Intersections of these sets need not belong to the system of contexts (nor complements of these sets). Thus the Boolean structure of the original first level description disappeared, but, nevertheless, it is present in the latent form. Point-sets $\{\omega_j\}$ are not "visible" at this level of description. For example, the random variable

$$\eta(\omega_j) = \gamma_j, j = 1, ..., 4, \ \gamma_i \neq \gamma_j, i \neq j,$$

is not an observable at the second level.

Such a model was discussed from positions of quantum logic, see, e.g., [22]. There can be provided a nice interpretation of these two levels of description. Let us consider a firefly in the box. It can fly everywhere in this box. Its locations are described by the uniform probability distribution $\mathbf{P}$ (on the σ-algebra of Borel subsets of the box). This is the first level of description. Such a description can be realized if the box were done from glass or if at every point of the box there were a light detector. All Kolmogorov random variables can be considered as observables.

Now we consider the situation when there are only two possibilities to observe the firefly in the box: 1) to open a small window at a point a which is located in such a way that it is possible to determine only either the firefly is in the section A_1 or in the section A_2 of the box; 2) to open a small window at a point b which is located in such a way that it is possible to determine only either the firefly is in the section B_1 or in the section B_2 of the box. In the first case I can determine in which part, A_1 or A_2, the firefly is located. In the second case I also can only determine in which part, B_1 or B_2, the firefly is located. But I am not able to look into both windows simultaneously. In such a situation the observables a and b are the only source of information about the firefly (reference observables). The Kolmogorov description is meaningless (although it is incorporated in the model in the latent form). Can one apply a quantum-like description, namely, represent contexts by complex probability amplitudes? The answer is to be positive. The set of contexts that permit the quantum-like representation consists of all subsets C such that $\mathbf{P}(A_i|C) > 0$ and $\mathbf{P}(B_i|C) > 0, i = 1, 2$ (i.e., for sufficiently large contexts). We have seen that the Boolean structure disappeared as a consequence of ignorance of information.

Finally, we emphasize again that the Växjö model is essentially more general. The set-theoretic representation need not exist at all.

4. Boolean and quantum logic

Typically the absence of the Boolean structure on the set of quantum propositions is considered as the violation of laws of classical logic, e.g., in quantum mechanics [23]. In our approach classical logic is not violated, it is present in the latent form. However, we are not able to use it, because we do not have complete information. Thus quantum-like logic is a kind of projection of classical logic. The impossibility of operation with complete information about a system is not always a disadvantages. Processing of incomplete set of information has the evident advantage comparing with "classical Boolean" complete information processing – the great saving of computing resources and increasing of the speed of computation. However, the Boolean structure cannot be violated in an arbitrary way, because in such a case we shall get a chaotic computational process. There should be developed some calculus of consistent ignorance by information. Quantum formalism provides one of such calculi.

Of course, there are no reasons to assume that processing of information through ignoring of its essential part should be rigidly coupled to a special class of physical systems, so called quantum systems. Therefore we prefer to speak about *quantum-like processing of information* that may be performed by various kinds of physical and

biological systems. In our approach quantum computer has advantages not because it is based on a special class of physical systems (e.g., electrons or ions), but because there is realized the consistent processing of incomplete information. We prefer to use the terminology QL-computer by reserving the "quantum computer" for a special class of QL-computers which are based on quantum physical systems.

One may speculate that some biological systems could develop in the process of evolution the possibility to operate in a consistent way with incomplete information. Such a QL-processing of information implies evident advantages. Hence, it might play an important role in the process of the natural selection. It might be that consciousness is a form of the QL-presentation of information. In such a way we really came back to Whitehead's analogy between quantum and conscious systems [26].

5. Supplementary ("Incompatible") Observables in the Växjö Model

Nowadays the notion of incompatible (complementary) observables is rigidly coupled to *noncommutativity.* In the conventional quantum formalism observables are incompatible iff they are represented by noncommuting self-adjoint operators $\hat{a}$ and $\hat{b} : [\hat{a}, \hat{b}] \neq 0$. As we see, the Växjö model is not from the very beginning coupled to a representation of information in a Hilbert space. Our aim is to generate an analogue (may be not direct) of the notion of incompatible (complementary) observables starting not from the mathematical formalism of quantum mechanics, but on the basis of the Växjö model, i.e., directly from statistical data.

Why do I dislike the conventional identification of *incompatibility with noncommutativity?* The main reason is that typically the mathematical formalism of quantum mechanics is identified with it as a physical theory. Therefore the quantum incompatibility represented through noncommutativity is rigidly coupled to the micro-world. (The only possibility to transfer quantum behavior to the macro-world is to consider physical states of the Bose-Einstein condensate type.) We shall see that some Växjö models can be represented as the conventional quantum model in the complex Hilbert space. However, the Växjö model is essentially more general than the quantum model. In particular, some Växjö models can be represented not in the complex, but in hyperbolic Hilbert space (the Hilbert module over the two dimensional Clifford algebra with the generator $j : j^2 = +1$).

Another point is that the terminology – incompatibility – is misleading in our approach. The quantum mechanical meaning of compatibility is the possibility to measure two observables, a and b *simultaneously.* In such a case they are represented by commuting operators. Consequently incompatibility implies the impossibility of simultaneous measurement of a and b. In the Växjö model there is no such a thing as fundamental impossibility of simultaneous measurement. We present the viewpoint that quantum incompatibility is just a consequence of information *supplementarity* of observables a and b. The information which is obtained via a measurement of, e.g., b can be non trivially updated by additional information which is contained in the

result of a measurement of a. Roughly speaking if one knows a value of b, say $b = y$, this does not imply knowing the fixed value of a and vice versa, see [14] for details.

We remark that it might be better to use the notion "complementary," instead of "supplementary." However, the first one was already reserved by Nils Bohr for the notion which very close to "incompatibility." In any event Bohr's complementarity implies *mutual exclusivity* that was not the point of our considerations.

Supplementary processes take place not only in physical micro-systems. For example, in the brain there are present supplementary mental processes. Therefore the brain is a (macroscopic) QL-system. Similar supplementary processes take place in economy and in particular at financial market. There one could also use quantum-like descriptions [24]. But the essence of the quantum-like descriptions is not the representation of information in the complex Hilbert space, but incomplete (projection-type) representations of information. It seems that the Växjö model provides a rather general description of such representations.

We introduce a notion of supplementary which will produce in some cases the quantum-like representation of observables by noncommuting operators, but which is not identical to incompatibility (in the sense of impossibility of simultaneous observations) nor complementarity (in the sense of mutual exclusivity).

Definition 2. *Let $a, b \in \mathcal{O}$. The observable a is said to be supplementary to the observable b if*

$$p^{a|b}(x|y) \neq 0, \tag{5.1}$$

for all $x \in X_a, y \in X_b$.

Let $a = x_1, x_2$ and $b = y_1, y_2$ be two dichotomous observables. In this case (5.1) is equivalent to the condition:

$$p^{a|b}(x|y) \neq 1, \tag{5.2}$$

for all $x \in X_a, y \in X_b$. Thus by knowing the result $b = y$ of the b-observation we are not able to make the definite prediction about the result of the a-observation.

Suppose now that (5.2) is violated (i.e., a is not supplementary to b), for example:

$$p^{a|b}(x_1|y_1) = 1, \tag{5.3}$$

and, hence, $p^{a|b}(x_2|y_1) = 0$. Here the result $b = y_1$ determines the result $a = x_1$.

In future we shall consider a special class of Växjö models in that the matrix of transition probabilities $\mathbf{P}^{a|b} = (p^{a|b}(x_i|y_j))_{i,j=1}^2$ is *double stochastic:* $p^{a|b}(x_1|y_1) + p^{a|b}(x_1|y_2) = 1; p^{a|b}(x_2|y_1) + p^{a|b}(x_2|y_2) = 1$. In such a case the condition (5.3) implies that

$$p^{a|b}(x_2|y_2) = 1, \tag{5.4}$$

and, hence, $p^{a|b}(x_1|y_2) = 0$. Thus also the result $b = y_2$ determines the result $a = x_2$.

We point out that for models with double stochastic matrix $\mathbf{P}^{a|b} = (p^{a|b}(x_i|y_j))_{i,j=1}^2$ the relation of supplementary is symmetric! In general it is not the case. It can happen that a is supplementary to b : each a-measurement gives us additional information updating information obtained in a preceding measurement of b (for any result $b = y$). But b can be non-supplementary to a.

Let us now come back to Example 1. The observables a and b are supplementary in our meaning. Consider now the classical Kolmogorov model and suppose that we are able to measure not only the random variables ξ_a and ξ_b – observables a and b, but also the random variable η. We denote the corresponding observable by d. The pairs of observables (d, a) and (d, b) are non-supplementary:

$$p^{a|d}(x_1|\gamma_i) = 0, \ i = 3, 4; \ p^{a|d}(x_2|\gamma_i) = 0, \ i = 1, 2,$$

and, hence,

$$p^{a|d}(x_1|\gamma_i) = 1, \ i = 1, 2; \ p^{a|d}(x_2|\gamma_i) = 1, \ i = 3, 4.$$

Thus if one knows , e.g., that $d = \gamma_1$ then it is definitely that $a = x_1$ and so on.

6. Test of Quantum-like Structure

We consider examples of cognitive contexts:

1). C can be some selection procedure that is used to select a special group S_C of people or animals. Such a context is represented by this group S_C (so this is an ensemble of cognitive systems). For example, we select a group $S_{\text{prof.math.}}$ of professors of mathematics (and then ask questions a or (and) b or give corresponding tasks). We can select a group of people of some age. We can select a group of people having a "special mental state": for example, people in love or hungry people (and then ask questions or give tasks).

2). C can be a learning procedure that is used to create some special group of people or animals. For example, rats can be trained to react to special stimulus.

We can also consider *social contexts.* For example, social classes: proletariat-context, bourgeois-context; or war-context, revolution-context, context of economic depression, poverty-context, and so on. Thus our model can be used in social and political sciences (and even in history). We can try to find quantum-like statistical data in these sciences.

We describe a mental interference experiment.

Let $a = x_1, x_2$ and $b = y_1, y_2$ be two dichotomous mental observables: x_1=yes, x_2=no, y_1=yes, y_2=no. We set $X \equiv X_a = \{x_1, x_2\}, Y \equiv X_b = \{y_1, y_2\}$ ("spectra" of observables a and b). Observables can be two different questions or two different types of cognitive tasks. We use these two fixed reference observables for probabilistic representation of cognitive contextual reality given by C.

We perform observations of a under the complex of cognitive conditions C :

$$p^a(x) = \frac{\text{the number of results } a = x}{\text{the total number of observations}}.$$

So $p^a(x)$ is the probability to get the result x for observation of the a under the complex of cognitive conditions C. In the same way we find probabilities $p^b(y)$ for the b-observation under the same cognitive context C.

As was supposed in axiom 1, cognitive contexts C_y can be created corresponding to selections with respect to fixed values of the b-observable. The context C_y (for

fixed $y \in Y$) can be characterized in the following way. By measuring the b-observable under the cognitive context C_y we shall obtain the answer $b = y$ with probability one. We perform now the a-measurements under cognitive contexts C_y for $y = y_1, y_2$, and find the probabilities:

$$p^{a|b}(x|y) = \frac{\text{number of the result } a = x \text{ for context } C_y}{\text{number of all observations for context } C_y}$$

where $x \in X, y \in Y$. For example, by using the ensemble approach to probability we have that the probability $p^{a|b}(x_1|y_2)$ is obtained as the frequency of the answer $a = x_1 = yes$ in the ensemble of cognitive system that have already answered $b = y_2 = no$. Thus we first select a sub-ensemble of cognitive systems who replies no to the b-question, $C_{b=no}$. Then we ask systems belonging to $C_{b=no}$ the a-question.

It is assumed (and this is a very natural assumption) that a cognitive system is "responsible for her (his) answers." Suppose that a system τ has answered $b = y_2 = no$. If we ask τ again the same question b we shall get the same answer $b = y_2 = no$. This is nothing else than *the mental form of the von Neumann projection postulate:* the second measurement of the same observable, performed immediately after the first one, will yield the same value of the observable).

Classical probability theory tells us that all these probabilities have to be connected by the so called *formula of total probability:*

$$p^a(x) = p^b(y_1)p^{a|b}(x|y_1) + p^b(y_2)p^{a|b}(x|y_2), \quad x \in X.$$

However, if the theory is quantum-like, then we should obtain [13] the formula of total probability with an interference term:

$$p^a(x) = p^b(y_1)p^{a|b}(x|y_1) + p^b(y_2)p^{a|b}(x|y_2) \tag{6.1}$$

$$+2\lambda(a = x|b, C)\sqrt{p^b(y_1)p^{a|b}(x|y_1)p^b(y_2)p^{a|b}(x|y_2)},$$

where the coefficient of supplementarity (the coefficient of interference) is given by $\lambda(a = x|b, C) =$

$$\frac{p^a(x) - p^b(y_1)p^{a|b}(x|y_1) - p^b(y_2)p^{a|b}(x|y_2)}{2\sqrt{p^b(y_1)p^{a|b}(x|y_1)p^b(y_2)p^{a|b}(x|y_2)}} \tag{6.2}$$

This formula holds true for *supplementary observables.* To prove its validity, it is sufficient to put the expression for $\lambda(a = x|b, C)$, see (6.2), into (6.1). In the quantum-like statistical test for a cognitive context C we calculate
$\lambda(a = x|b, C) =$

$$\frac{p^a(x) - p^b(y_1)p^{a|b}(x|y_1) - p^b(y_2)p^{a|b}(x|y_2)}{2\sqrt{p^b(y_1)p^{a|b}(x|y_1)p^b(y_2)p^{a|b}(x|y_2)}}.$$

An empirical situation with $\lambda(a = x|b, C) \neq 0$ would yield evidence for quantum-like behaviour of cognitive systems. In this case, starting with (experimentally calculated) coefficient of interference $\lambda(a = x|b, C)$ we can proceed either to the conventional Hilbert space formalism (if this coefficient is bounded by 1) or to so called

hyperbolic Hilbert space formalism (if this coefficient is larger than 1). In the first case the coefficient of interference can be represented in the trigonometric form $\lambda(a = = x|b, C) = \cos\theta(x)$, Here $\theta(x) \equiv \theta(a = x|b, C)$ is the phase of the a-interference between cognitive contexts C and $C_y, y \in Y$. In this case we have the conventional formula of total probability with the interference term:

$$p^a(x) = p^b(y_1)p^{a|b}(x|y_1) + p^b(y_2)p^{a|b}(x|y_2) \tag{6.3}$$

$$+2\cos\theta(x)\sqrt{p^b(y_1)p^{a|b}(x|y_1)p^b(y_2)p^{a|b}(x|y_2)}.$$

In principle, it could be derived in the conventional Hilbert space formalism. But we chosen the inverse way. Starting with (6.3) we could introduce a "mental wave function" $\psi \equiv \psi_C$ (or pure quantum-like mental state) belonging to this Hilbert space. We recall that in our approach a mental wave function ψ is just a representation of a cognitive context C by a complex probability amplitude. The latter provides a Hilbert representation of statistical data about context which can be obtained with the help of two fixed observables (reference observables).

7. Wave Function Representation of Cognitive Contexts

Let C be a cognitive context. We consider only cognitive contexts with trigonometric interference for *supplementary mental observables* a and b. The interference formula of total probability (6.1) can be written in the following form: $p_C^a(x) =$

$$\sum_{y \in Y} p_C^b(y)p^{a|b}(x|y) + 2\cos\theta_C(x)\sqrt{\Pi_{y \in Y}p_C^b(y)p^{a|b}(x|y)} \tag{7.1}$$

By using the elementary formula: $D = A + B + 2\sqrt{AB}\cos\theta = |\sqrt{A} + e^{i\theta}\sqrt{B}|^2, A, B > 0$, we can represent the probability $p_C^b(x)$ as the square of the complex amplitude:

$$p_C^a(x) = |\psi_C(x)|^2 \tag{7.2}$$

where

$$\psi(x) \equiv \psi_C(x) = \sum_{y \in Y} \sqrt{p_C^b(y)p^{a|b}(x|y)}e^{i\xi_C(x|y)}. \tag{7.3}$$

Here phases $\xi_C(x|y)$ are such that $\xi_C(x|y_1) - \xi_C(x|y_2) = \theta_C(x)$. We denote the space of functions: $\psi : X \rightarrow \mathbf{C}$ by the symbol $E = \Phi(X, \mathbf{C})$. Since $X = \{x_1, x_2\}$, the E is the two dimensional complex linear space. Dirac's $\delta-$functions $\{\delta(x_1 - x), \delta(x_2 - x)\}$ form the canonical basis in this space. For each $\psi \in E$ we have $\psi(x) = \psi(x_1)\delta(x_1 - - x) + \psi(x_2)\delta(x_2 - x)$.

Denote by the symbol $\mathcal{C}^{\text{tr}}$ the set of all cognitive contexts having the trigonometric statistical behaviour (i.e., $|\lambda| \leq 1$) with respect to mental observables a and b. By using the representation (7.3) we construct the map $\tilde{J}^{a|b} : \mathcal{C}^{\text{tr}} \rightarrow \tilde{\Phi}(X, \mathbf{C})$, where $\tilde{\Phi}(X, \mathbf{C})$ is the space of equivalent classes of functions under the equivalence relation: φ equivalent ψ iff $\varphi = t\psi, t \in \mathbf{C}, |t| = 1$. We point out that if the matrix of transition probabilities for the reference observables is double stochastic, then $a|b$-representation is equivalent to the $b|a$-representation. In general it is not the case.

8. Quantum-like Processing of Information in Brain

The brain is a huge information system that contains millions of elementary mental states . It could not "recognize" (or "feel") all those states at each instant of time t. Our fundamental hypothesis is that the brain is able to create the QL-representations of mind. At each instant of time t the brain creates the QL-representation of its mental context C based on two supplementary mental (self-)observables a and b. Here $a = (a_1, ..., a_n)$ and $b = (b_1, ..., b_n)$ can be very long vectors of compatible (non-supplementary) dichotomous observables. The reference observables a and b can be chosen (by the brain) in different ways at different instances of time. Such a change of the reference observables is known in cognitive sciences as a *change of representation.*

A mental context C in the $a|b-$ representation is described by the mental wave function ψ_C. We can speculate that the brain has the ability to feel this mental field as a distribution on the space X. This distribution is given by the norm-squared of the mental wave function: $|\psi_C(x)|^2$.

In such a model it might be supposed that the state of our consciousness is represented by the mental wave function ψ_C. The crucial point is that in this model consciousness is created through neglecting an essential volume of information contained in subconsciousness. Of course, this is not just a random loss of information. Information is selected through the algorithm of the probabilistic representation, see (7.3): a mental context C is projected onto the complex probability amplitude ψ_C.

The (classical) mental state of sub-consciousness evolves with time $C \to C(t)$. This dynamics induces dynamics of the mental wave function $\psi(t) = \psi_{C(t)}$ in the complex Hilbert space.

Further development of our approach (which we are not able to present here) induces the following model of brain's functioning [25]:

The brain is able to create the QL-representation of mental contexts, $C \to \psi_C$ (by using the algorithm based on the formula of total probability with interference).

9. Brain as Quantum-like Computer

The ability of the brain to create the QL-representation of mental contexts induces functioning of the brain as a quantum-like computer.

The brain performs computation-thinking by using algorithms of quantum computing in the complex Hilbert space of mental QL-states.

We emphasize that in our approach the brain is not quantum computer, but a QL-computer. On one hand, a QL-computer works totally in accordance with the mathematical theory of quantum computations (so by using quantum algorithms). On the other hand, it is not based on superposition of individual mental states. The complex amplitude ψ_C representing a mental context C is a special probabilistic representation of information states of the huge neuronal ensemble. In particular, the brain is a *macroscopic* QL-computer. Thus the QL-parallelism (in the opposite to conventional quantum parallelism) has a natural realistic base. This is real parallelism in the working of millions of neurons. The crucial point is the way in which this

classical parallelism is projected onto dynamics of QL-states. The QL-brain is able to solve NP-problems. But there is nothing mysterious in this ability: an exponentially increasing number of operations is performed through involving of an exponentially increasing number of neurons.

We point out that by coupling QL-parallelism to working of neurons we started to present a particular ontic model for QL-computations. We shall discuss it in more detail. Observables a and b are self-observations of the brain. They can be represented as functions of the internal state of brain ω. Here ω is a parameter of huge dimension describing states of all neurons in the brain: $\omega = (\omega_1, \omega_2, ..., \omega_N)$:

$$a = a(\omega), b = b(\omega).$$

The brain is not interested in concrete values of the reference observables at fixed instances of time. The brain finds the contextual probability distributions $p_C^a(x)$ and $p_C^b(y)$ and creates the mental QL-state $\psi_C(x)$, see the QL-representation algorithm (7.3). Then it works with the mental wave function $\psi_C(x)$ by using algorithms of quantum computing.

Conclusion: *We presented a consistent approach to QL-information representation as incomplete information representation.*

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Quantum Bit String Comparator: Circuits and Applications

Quantum computation has attracted much attention since it was shown by Shor and Grover the possibility to implement quantum algorithms able to realize, respectively, factoring and searching in a faster way than any other known classical algorithm. In particular, it is possible to use Grover's algorithm, taking profit of its ability to find a specific value in an unordered database, to find, for example, the zero of a logical function or the minimal or maximal value in a database. Here we show quantum algorithms to solve those cited problems. The solution requires the use of a quantum bit string comparator. This quantum circuit compares two quantum states and identifies if they are equal or, otherwise, which of them is the largest. Moreover, we also show the quantum bit string comparator allow us to implement conditional statements in quantum computation, a fundamental structure for designing of algorithms.

1. Introduction

The Grover's quantum search algorithm is a celebrated result in quantum computation that proves that quantum information properties (superposition) can improve the speedup of finding a specific value within an unordered database. In this case, no technique using data structures can be used and only sequential tentative can be realized. Computationally, the quantum search is proved to get in average $O(N^{1/2})$ operations (in comparison with the $O(N)$ classical operations), which indicates a quadratic speed-up [1–3]. Even though this improvement can be considered minor than other quantum algorithms, Shor [4] and Deutsch-Jozsa[5] algorithms are exponentially better than their classical counterparts, the fact is that searching is fundamental in computer science having a large amount of applications. In addition, no classical algorithm can be more efficient than Grover algorithm, that is, the quantum search algorithm is as efficient as the best search algorithm could be. The basic reason that allows this performance is the smart use of the quantum superposition which means that all states can be processed at once (in contrast with the combinatory explosion of the classical alternatives). Basically, during the processing, the database, initially an equally weighted superposition of all possible states, converges to a state that can also be a superposition, but

containing only the states that are solutions of the problem, named marked states. There are several works on variations of Grover's algorithm [6,7], entanglement measures based on the Grover' algorithm [8,9] and implementation of Grover's algorithm [10,11]. Here, our goal is to show how to solve some interesting mathematical problems using the Grover's algorithm with an oracle based in a quantum circuit that compares two quantum states, representing binary strings, and identifies if they are equal or not and, in this last case, which of them is the largest (or the lowest). The circuit that makes the comparison is named quantum bit string comparator, QBSC. Furthermore, we show how to use the QBSC to construct quantum algorithms that employ conditional statements.

2. Quantum circuits for the quantum bit string comparator

Given two n-partite of qubits quantum states $|a\rangle|b\rangle$ the quantum bit string comparator is a unitary evolution U_{CMP} that works as shown in (1)

$$U_{CMP}|a\rangle|b\rangle|0^{\otimes m}\rangle|0\rangle|0\rangle = |a\rangle|b\rangle|\psi\rangle|x\rangle|y\rangle. \tag{1}$$

In (1) there are $m+2$ ancillas at the input, $|\psi\rangle$ is a m qubit output state that has not important information and the last two qubits carry the comparison information. For example, if $a=b$ then $x=y=0$, if $a>b$ then $x=1$ and $y=0$, and if $a<b$ then $x=0$ and $y=1$. The evolution shown in (1) can be realized using the quantum circuit shown in Fig. 1 (for three qubits strings). It is able to compare two binary strings (having the same number of bits) identifying, by the measurement of two qubits, if they are equal or, if they are different, which of them is the largest (or the lowest).
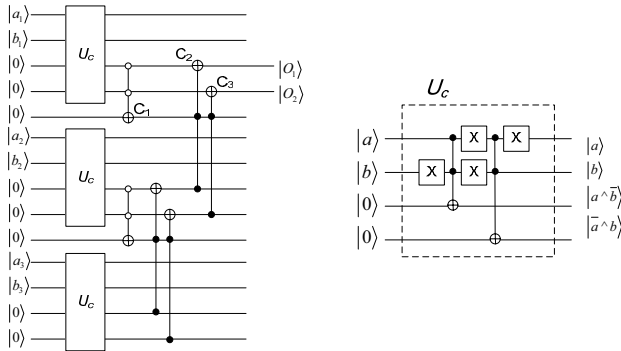
Fig. 1. Quantum circuit for comparison of two strings of three qubits: $|a\rangle=|a_1\rangle|a_2\rangle|a_3\rangle$ and $|b\rangle=|b_1\rangle|b_2\rangle|b_3\rangle$

The quantum circuit proposed makes the comparison of two strings of three qubits, but the generalization to any number of qubits is straightforward. Basically, the quantum circuit compares the strings bit-to-bit from the left (most significant bit) to the right (less significant bit). In a measurement of the outputs (O_1 and O_2), if $O_1=1$ and $O_2=0$ then $a>b$; if $O_1=0$ and

O_2=1 then $a<b$; at last, if O_1=0 and O_2=0 then $a=b$. Initially, the comparison between the first bit of each string is dominant, that is, if they are different, then the outputs will be $O_1=a_1$ and $O_2=b_1$. If they are equal ($a_1=b_1$) the comparison between the second bit of each string will be dominant, that is, if they are different, then the outputs will be $O_1=a_2$ and $O_2=b_2$. If the second bits are also equal, the comparison between the third bits of each string will be dominant and so on. In the circuit of Fig. 1 the transfer of dominion from one position of the string to the next is realized by the Toffoli gate C_1 (activated in zero) and the Toffoli gates C_2 and C_3. Obviously, only the less significant bit does not have the dominion transfer circuit. The following examples, shown in Table 1, will make clear the functioning of the circuit (for simplicity it will be considered the comparison of two states of two qubits, but the result is directly generalized for any number of qubits).

Table 1. Examples of the output of the quantum bit string comparator for two strings of two qubits at the inputs.

$|a\rangle$	$|10\rangle$	$|00\rangle$	$|10\rangle$	$|11\rangle$	$|01\rangle$
$|b\rangle$	$\alpha|00\rangle+\beta|01\rangle$	$\alpha|01\rangle+\beta|10\rangle$	$\alpha|00\rangle+\beta|11\rangle$	$\alpha|01\rangle+\beta|11\rangle$	$\alpha|01\rangle+\beta|11\rangle$
O_1	$|1\rangle$ (1)	$|0\rangle$ (1)	$|1\rangle$ ($|\alpha|^2$)	$|1\rangle$ ($|\alpha|^2$)	$|0\rangle$ (1)
O_2	$|0\rangle$ (1)	$|1\rangle$ (1)	$|1\rangle$ ($|\beta|^2$)	$|0\rangle$ (1)	$|1\rangle$ ($|\beta|^2$)

In Table 1, the number inside the parenthesis besides the qubit means the probability of the output to be that qubit. For example, comparing $|a\rangle=|11\rangle$ with $|b\rangle=\alpha|01\rangle+\beta|11\rangle$, with probability $|\alpha|^2$ $a>b$ and, hence, $|O_1O_2\rangle=|10\rangle$. On the other hand, with probability $|\beta|^2$ $a=b$ and, hence, $|O_1O_2\rangle=|00\rangle$. Hence, in this case, the output state is $|O_1O_2\rangle=(\alpha|1\rangle_1+\beta|0\rangle_1)|0\rangle_2$. Another quantum circuit for the QBSC, based on subtractions, named NKO, can be as shown in Fig. 2 [12].
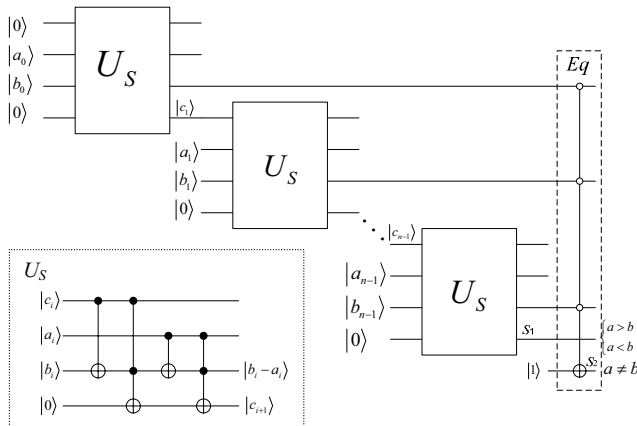

Figure 2 - Quantum circuit for comparison of two strings of qubits using subtractions

In order to compare the quantum circuits shown in Figs. 1 and 2, we realized a complexity analysis. Since the construction of any quantum circuit can be done using single qubit gates (Sq) and CNOT gates (Cn), the cost of the circuits QBSC and NKO is calculated based on the unitary cost of those universal gates. The unitary costs are defined by: 1) Cost of Sq = $1u$. 2) Cost of Cn = $1d$. For example, the Swap and Toffoli gates have the following costs:

- The Swap (Sw) gate can be constructed using three CNOT gates, hence, it costs $3d$;
- The Toffoli (Tof) gate can be constructed without ancilla [13] as shown in Fig. 3. It costs Three Cn, two Sw and four Sq, then, it costs $9d+4u$.
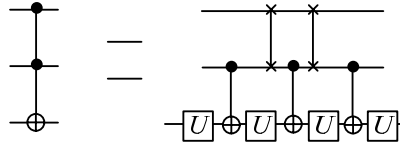

Figure 3. Toffoli gate implemented using only single-qubit gates and CNOT gates, without ancillas.

Thus, the final cost to construct a n-qubit QBSC is presented in Table 2.

Table 2. Construction cost of QBSC circuit.

Gate	Components	Unitary Cost	Quantity
Uc	$2\ Tof + 2\ Sw + 4\ Pu$	$24d+12u$	n
C_1	$1\ Tof + 4\ Pu$	$9d+8u$	$n-1$
C_2	$8\ Sw + 1\ Tof$	$33d+4u$	$n-1$
C_3	$8\ Sw + 1\ Tof$	$33d+4u$	$n-1$

The total n-qubit QBSC cost is [$99(n-1)+24$] CNOTs and [$28(n-1)+12$] single-qubit gates.

To realize the NKO complexity analysis, we assume that the quantum gate to verify the equality (Eq) is constructed using Swap gates to order the qubits and one MCNOT gate with n-control qubits. The two low cost way to implement the MCNOT with n-control qubits [14] are shown in Table 3 with their respective costs.

Table 3. Cost to implement a MCNOT gate with n-control qubits.

Gate	Ancilla qubits	Number of Toffolis	Total cost
MCNOT1	1	$32n-96$	$288n{\cdot}d-864d+128n{\cdot}u-384u$
MCNOT2	$n-2$	$16n-32$	$144n{\cdot}d-288d+64n{\cdot}u-128u$

One can construct the NKO circuit using MCNOT1 or MCNOT2. The construction cost of the NKO components are presented in Table 4.

Table 4. Cost to implement a NKO circuit

Gate	Components	Unitary cost	Quantity
Us	$2\ Sw + 2\ Cn + 2\ Tof$	$17d+4u$	n
$Eq1$	$n^2\ Sw + 2n\ Pu + McN1$	$3n^2d+288n{\cdot}d-864d+130n{\cdot}u-384u$	1
$Eq2$	$n^2\ Sw + 2n\ Pu + McN2$	$3n^2d+144n{\cdot}d-288d+66n{\cdot}u-128u$	1

Using Table 3, we see that NKO1 (NKO with $Eq1$, that uses MCNOT1) has total cost of $[3n^2+305n-864]$ CNOTs and $[134n-384]$ single-qubit gates. The NKO2 (NKO with $Eq2$, that uses MCNOT2) has total cost of $[3n^2 +161n-288]$ CNOTs and $[70n-128]$ single-qubit gates. Therefore, the creation of NKO circuit requires more resources than the creation of QBSC circuit. This happen because of the MCNOT used by NKO. The Figures 4 and 5 show, respectively, the graphics of the number of CNOT gates and single qubit gates required by QBSC and KNO in order to build a n-qubit comparison quantum circuit.
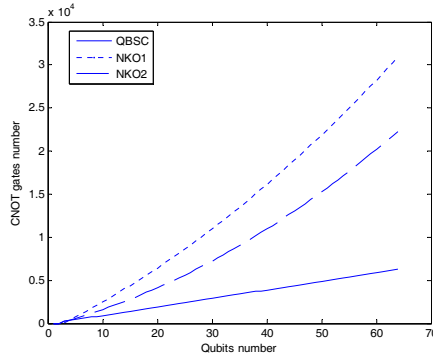
Figure 4. Number of CNOTs versus number of qubits for QBSC, NKO1 and KNO2.
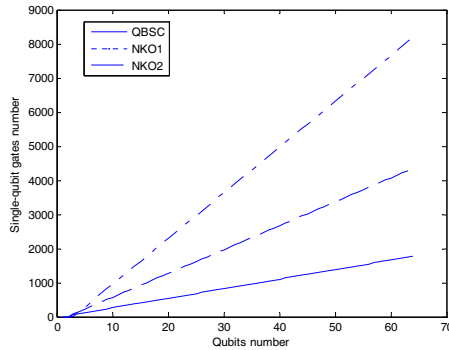
Figure 5. Number of single-qubit gates versus number of qubits for QBSC, NKO1 and KNO2.

Another point to be considered is the number of ancillas needed. For the QBSC are necessary $3n$-1, as can be calculated observing Fig. 1. The NKO1 needs $n+3$ ancillas. Observing Fig. 2 one counts $n+2$, the last one comes from the implementation of the MCNOT and it is not shown in Fig. 2. Finally, the NKO2 uses $2n$ ancillas.

The last parameter to be considered is the degree of parallelism, that is, how compact the comparators can be constructed. The larger the number of gates that can be simultaneously used the faster is the program execution. In QBSC, the comparison between the pairs of qubits can be parallelized, that is, every gates Uc and C_1 can be processed at the same time.

2. Applications of the quantum bit string comparator as an oracle in Grover's algorithm

There are several important applications of the comparison of binary strings in quantum computation. Let us firstly discuss the use of the QBSC as an oracle in the Grover's quantum search algorithm. An example of 4 qubits is shown in Fig. 6, but a generalization for any number of qubits is straightforward.
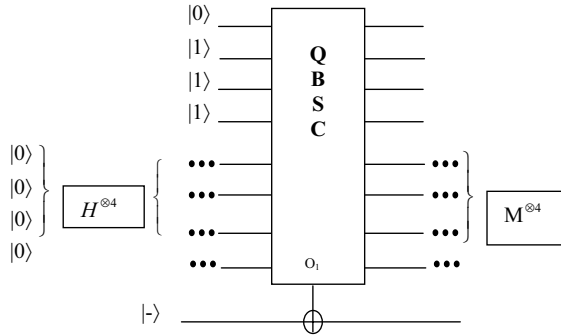

Figure 6 - QBSC circuit as an oracle in a Grover search algorithm of four qubits.
H- Hadamard gate. M – Measurer.

For the circuit shown in Fig. 6, the task is to search in the database words of four bits larger than "0111". This is clearly a typical case of multiple marked states and, hence, the output of Grover's algorithm will be a superposition of the all possible solutions. The reference state $|0111\rangle$ works as string $|a\rangle$ while the database is $|b\rangle$. If the initial state of Grover's algorithm is $(1/4)\sum_{i=0}^{15}|i\rangle$ then the output state will be:

$$\frac{\left(|8\rangle+|9\rangle+|10\rangle+|11\rangle+|12\rangle+|13\rangle+|14\rangle+|15\rangle\right)}{2\sqrt{2}} \qquad (2)$$

where the decimal representation has been used for simplification. If instead of search for states larger than $|0111\rangle$ one was looking for states lower than $|0111\rangle$, then O_2 would be used instead of O_1 (the reference is $|a\rangle$). Let us now suppose that the goal is to find the minimal value in the database. In order to find the minimal value the quantum circuit shown in Fig. 4 has to be used to activate the lowest CNOT of Grover's quantum circuit.

Using the circuit of Fig. 7, the oracle will recognize strings lower or equal than the reference. The algorithm to find the minimum is as follows [15]: Initially, one value of the database is randomly chosen. This value will be used for comparison (string $|a\rangle$). The algorithm runs and, at end, the result of the measurement will be one of the members of the database lower or equal than the initial value used. The result of the measurement will now be used as the new value to be compared. The process is repeated till the result of the measurement does not change anymore. If one is looking for the minimal of a function *f*, represented by the

unitary evolution U_f, then the quantum circuit shown in Fig. 8 represents the complete oracle circuit.
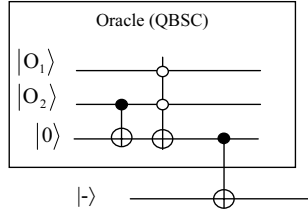
Figure 7. Control of the lowest CNOT of Grover's quantum circuit in order to find the minimal value in a database using the quantum comparator circuit as oracle.
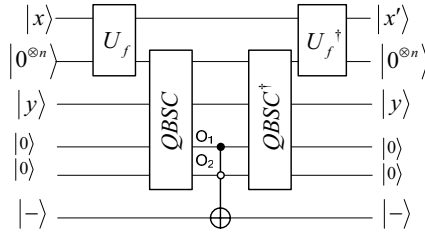
Figure 8. Oracle circuit with QBSC for finding the minimal value of the function f.

In Fig. 8, $|x\rangle$ is the database, $|y\rangle$ is the present "minimal value" that works as reference and the operation U_f acts in the following way: $U_f|x\rangle|0^{\otimes n}\rangle=|x\rangle|f(x)\rangle$.

Another interesting application is the problem of inverting a function, that is, given y what is the x such that $y=f(x)$. The unitary transformation U_f represents the function whose argument one wishes to find. In order to solve this problem, almost the same quantum circuit of Fig. 8 can be used, the difference is the Tofolli gate, that now has to be activated only when $O_1=O_2=0$ as shown in Fig. 9.
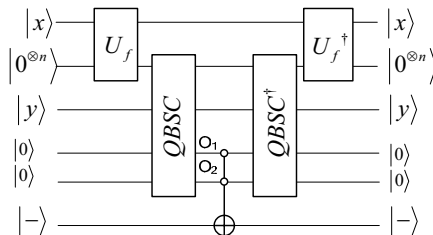
Figure 9. Oracle circuit with QBSC used to invert the function f.

Given a y, the oracle in Fig. 9 marks only those states $|x\rangle$ the obeys the condition $f(x)=y$. In particular, if $|y\rangle=|0^{\otimes n}\rangle$, then the oracle will recognize only the zero of the function f.

Another important question is the search of intervals. For example, given the constants y, α and β, what are the values of x for which $y-\beta<f(x)<y+\alpha$? The oracle to be used in the solution of this kind of problem is shown in Fig. 10.
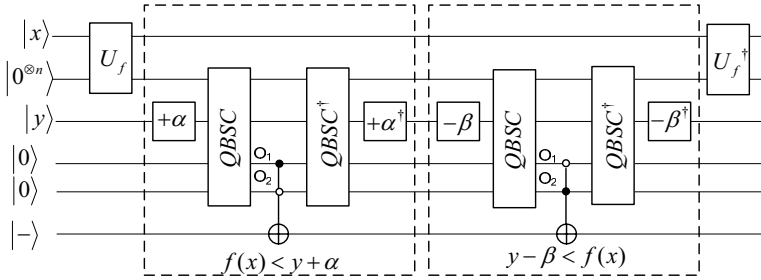
Figure 10. Oracle with QBSC for searching of the values of x such $y-\beta< f(x) < y+\alpha$.

In the quantum circuit in Fig. 10, the $+\alpha$ and $-\beta$ gates, whose ancillas are not shown, realize, respectively, the sum of α and subtraction of β. In Fig. 11.a-c it is shown for a fictitious example the change of the sign of the amplitudes before the first QBSC (*a*), after the first QBSC (*b*) and after the second QBSC (*c*).
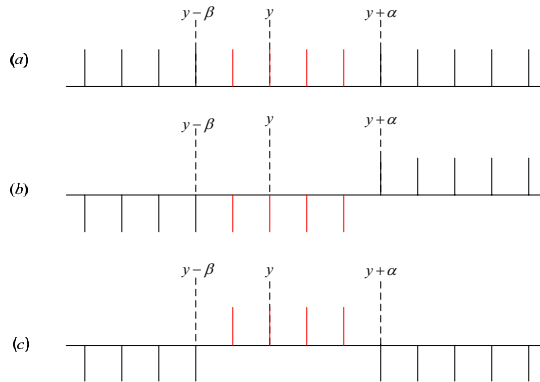
Figure 11. Change of the signs of the amplitudes during operation of the oracle shown in Fig. 10.

3. Conditional statements in quantum computation

In general, the QBSC expands the notion of controlled operation. Using the QBSC, controlled operations of the type U^C, where C is a conditional statement, can be constructed. In this case, the operator U is applied to a set of qubits only if the conditional statement C is true.

This last can be anyone of the type $a>b$, $a<b$, $a \geq b$, $a \leq b$, $a=b$ and $a \neq b$. For instance, using again the Grover's algorithm as scenario, we can implement the following piece of software: If $|a\rangle > |b\rangle$ then search for solution S_1, otherwise, search for solution S_2. For an oracle based on n-CNOTS, the quantum circuit for a four bit problem is as shown in Fig. 12.
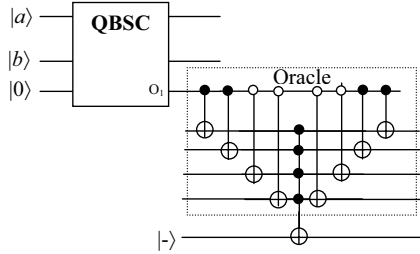
Figure 12. Implementation of the conditional statement: If $a>b$ then search for solution $S_1=|0011\rangle$, otherwise, search for solution $S_2=|1100\rangle$.

In Fig. 12, if $a>b$ the Grover algorithm will search for $|0011\rangle$, otherwise the algorithm will search for $|1100\rangle$.

4. Conclusions

The quantum bit string comparator enables the implementation of quantum algorithms using conditional statements, a fundamental structure for designing of algorithms. This enlarges the number of applications where quantum algorithms can be used and, at the same time, it brings close to quantum programmers successful techniques used in classical computation based on comparisons. Furthermore, the use of the QBSC with Grover algorithm gives us power to solve some mathematical problems of the type presented in this work, as well open the possibility to create quantum algorithm with very specific tasks. For example, constructing a database composed only of prime numbers it is possible, using the QBSC and Grover algorithm, to search for an even number that does not satisfy Goldbach's conjecture (all even number larger than two can be written as the sum of two prime numbers).

Acknowledgements

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Genetic simulation of quantum dynamics by the principle of quantum state selection[*]

The simple genetic algorithm is proposed for the simulation of quantum many body dynamics. It uses the selection of entangled quantum states and has the inbuilt absolute decoherence that comes from the limitation of classical memory. It is shown how this selection model can be applied to the problem of molecular association in chemical reactions.

1. Introduction and background

Algorithmic approach to quantum theory was proposed by the author in previous works (see [3], [4]). It is based on our firm conviction that the effective classical algorithms with expert estimations of a user represent the sufficient tool for the complete description of the Nature on any levels including quantum theory. The key requirement in this approach is the simplicity and the transparency of algorithms which are designed for the simulation of main processes in the micro-world. The expected advantage of algorithmic approach comes from its possibility to give the effective algorithms in cases when the standard quantum theory gives no algorithms for many of such processes, and just here we can expect the advantage of algorithmic approach over the standard Copenhagen quantum theory.

The first example can come from chemistry, where the application of quantum methods has the long history. Nevertheless, quantum chemistry takes up stationary electronic configurations, conformations of molecules and bound energies only, and there is no robust chemical simulator. This situation is not random, because there is no full quantum description of real dynamical processes. Shredinger equation is not applicable even to the simplest chemical reaction like the capture of a free electron by the Coulomb field of a proton. Here the probability to obtain the electron in state 1s does not change in time that makes the capture impossible. In the reality the emission of free photons always plays the key role in the reactions of association of molecules. Just the emitted photons take off the energy for the moving atoms that makes possible their joint in the molecule. Unfortunately, quantum electrodynamics (QED) gives us no robust algorithms for such processes as well. QED leads to the divergence of sums for amplitudes and there is no completely satisfactory method to

avoid it. Even if such a method is found QED is not applicable to chemistry due to the more fundamental reason than the divergence of sums. QED is the part of quantum theory and hence it inherits its basic drawback: the principal absence of the integral description of quantum evolution. Unitary dynamics in quantum theory is strictly separated from the measurements, and quantum theory factually is the theory of unitary dynamics whereas for the full description of chemistry we manage with the both these types of dynamics. The account of photons in chemical reactions has no sense without some certain supposition about when the collapse of quantum state vector happens. Just this supposition lies beyond the framework of quantum theory, and this deprives the models of chemical reactions the status of exact theory.

The wish to describe chemistry leads us to the necessity to extend the methods of quantum theory to the dynamics of many particle processes. My opinion is that such an extension means the modification of the mathematical apparatus of quantum theory, namely we must use algorithmic approach instead of analytic and algebraic methods (see the previous discussion in [7]). Only this radical step makes possible to build the consistent description of chemical reactions.

The reason that the robust description of chemical reactions must unavoidably have quantum character lies in the fact that the essence of these reactions has quantum nature, namely, it is based on the fundamental notion of entangled states. In this paper I represent the model of chemistry where the basic element is quantum entanglement between the particles participating in the reaction. In general sense, this gives the new argument for algorithmic approach. In practical sense for those, who are looking for the robust algorithms this gives the good starting point for elaboration of effective algorithms for the simulating of chemical reactions.

2. Method of collective behavior

The method of collective behavior represents the good alternative for the algebraic description of quantum one particle evolution. The discussion about the previous versions of this approach (Bohm method) can be found in [7], [11]. The conventional matrix algebra leads to the tremendous non effective usage of computational resources.

the computational difficulties arise already for one quantum particle. Let its configuration space be divided to N elements. It means that the space of quantum states has the dimensionality N. If we apply the matrix algebra in any form for computations we force the computer to process all trajectories of the system passing through all N basic states. In the simplest case it is expressed in the multiplication of unitary matrices of the time evolution. The mean value of the module of matrix element is $1/\sqrt{N}$. If all the interference arising in the evolution of the system is constructive we would obtain the resulting matrix which coefficients are about $N \, 1/(\sqrt{N}\sqrt{N} = 1$, whereas they must be of the order $1/\sqrt{N}$. It means that the bulk of interference is destructive and the huge portion of the computational recourse is spent to verify only that there is no particle in the considered point. The computational methods of matrix algebra when applied to quantum mechanics a priori require the no efficient expenses of the computational resources. Such methods factually realize Ryman

scheme of integration for Shredinger equation that is based on the division of the configuration space to finite elements.

We propose the alternative approach corresponding to Lebeg scheme of integration. We take as the basic elements the point wise samples of the considered particle so that each sample will represent the whole particle in one point. The total number of samples must not be large and its dynamics must be the good approximation of the quantum dynamics of the initial particle. Our main aim is to avoid the huge non effective expenses of the computational resources featured to matrix algebra. After the developing of this technique for one quantum particle we could hope to apply this method for many quantum particles as well.

This method of representation of quantum particle by its samples we call the method of collective behavior. It realizes the requirement of strict economy of the computational resources, which is the basic principle of algorithmic approach. The requirement of maximal economy of the computational resources is not only esthetic. This requirement allows to build the models in which decoherence is inbuilt feature of the model but not an axiom as in the Copenhagen quantum mechanics. In is shown in [3] how this requirement gives us the classical urn scheme for Born distribution of probability for the results of quantum measurements.

Here we give the interpretation of the dynamics of one quantum particle by means of collective behavior. The cost that will be paid for the economy of the computational resources is the necessity to build the algorithm by means of mechanism of interaction between the samples of particle, not by the differential equations. For the method of collective behavior it is impossible to build the adequate differential equation. However, this situation has the positive sides as well, beyond economical computations. The model of quantum dynamics becomes nearer to classical than in the standard approach that makes possible its visual representation.

The proposed approach is the direct generalization of diffusion Monte Carlo method to the case of the time dependent solution of Shredinger equation. The known fact that DMC gives the most exact approximation of stationary wave functions among all computational methods inspires optimism in the practical application of the method of collective behavior for more complex problems.

3. Dynamical diffusion swarm

Here we define the main instrument of quantum simulation: dynamical diffusion swarm. This object generalizes two well known notions: the ensemble of point wise particles from DMC method, and the ensemble of particles with the interaction induced by some classical Hamiltonian $H(r, p)$. Particles from DMC have no speeds and they are designed for the computation of stationary states for which they give the best approximation. The density of particles ρ for the ensembles with classical Hamiltonian depends on the coordinate r and on the impulse p; it obeys Liouvill equation

$$\frac{d\rho}{dt} = -\{\rho, H\}.$$

The behavior determined by this equation cannot simulate quantum evolution with the admissible accuracy because it does not give principle quantum phenomena like Rabi oscillation or quantum spectra. Hence, for the simulation of quantum mechanics we must admit some elements of behavior of the samples which do not follow from the classical physics.

The next analog of the dynamical diffusion swarm is Calder Legett model for the partial decoherence of quantum particle in which the particle is considered as interacting with the bath of harmonic oscillators. This interaction gives some random speed to the particle. However, such a model is based on standard formalism whereas the dynamical diffusion swarm is designed to replace this formalism.

Why the dynamical diffusion swarm is better than the immediate solution of Shredinger equation ? In this solution we factually use Riemann schem of integration. We must perform computations of the wave function on the whole configuration space independently on the degree of constructiveness of the interference. Here on the main part of the space where the interference is destructive and the wave function factually equals zero we are forced to spend the computational recourse only to verify this. The dynamical diffusion swarm, in contrast, realizes the more general Lebeg scheme og integration. In this case the diffusion dynamics results in that the samples will concentrate in the areas of constructive interference themselves and we avoid the non effective expenses of the computational resources. This is the fundamental advantage of the diffusion dynamics. We will see that the cost for this is the non uniform dependence of diffusion rate on the grain of the length δx in contrast to the standard diffusion where the rate is uniform.

We proceed with the definitions. We call the swarm the finite set S consisting n identical point wise particles each of which $s \in S$ has its own coordinates and impulse $x(s),\ p(s) \in R^3$. In the method of collective behavior one quantum particle of the mass M and charge Q is represented by the swarm S each member $s \in S$ of which has the mass $m = M/n$ and the charge $q = Q/n$. The elements of this swarm are called the samples of this quantum particle. We suppose that the total number of samples n is so large that the swarm can be used as the approximation of the continuous media. E.g., if we need use the smaller and smaller spatial grain some samples will always occur in each spatial cell. But the dispersion of speeds will grow when the grain decreases, and we will have the separate swarm for each spatial grain δx.

The choice of spatial grain is closely connected with by the definition what object must be considered as quantum particle. Thiis definition in turn depends on the concrete problem and quantum particles are not necessary elementary in the sense of theoretical physics. The definition what must be treated as a particle presumes the choice of the typical length ΔX and the time ΔT, so that the size of particle is much lesser than ΔX, e.g. it can be treated as point wise, and the time interval ΔT is not less than the typical time of the processes we are interested in. Let us agree that the typical mean speeds of the considered shifts are much lesser than some limit speed of all movements c. For example, an atom can be treated as a point wise particle in he processes with $\Delta X > 10^{-8}m$ and $\Delta T > 10^{-10}s$. If we decrease the value of typical lengths and times then to obtain the right picture we must consider the

different set of elementary particles, for example, the separate nucleus and electrons inside of atom. If we fix ΔX and ΔT, then to obtain the dynamical picture we must define the smaller segments δx, δt, which will represent the elementary steps of the video film and which, however, must be much greater than the typical lengths and times $\tilde{\Delta}X$, $\tilde{\Delta}T$ of the more fundamental processes then the considered one (the gap between the different fundamental processes can be about 10^{-20}, that always allows to make this separation). Also in the same process with the fixed energy the times and lengths depends on masses. The separation of particles by their masses makes possible to consider for the bulk of processes in electrodynamics only electrons because the typical distances of flight of protons are to 1800 times smaller. We can then treat the chosen values ΔX, ΔT as the size of imaginary screen and the length of video film, and δx, δt as the grain of spatial resolution of screen and! the tim e of showing of one card in the film. We choose δx and δt maximal so that our film will be informative. After this choice the conclusion can be done about what particle should be treated as quantum and what as classical. For this the typical values of their action $a = M(\Delta X)^2/\Delta T$ should be compared with Plank constant h. If $a < h$ then the particle should be treated as quantum, otherwise as classical. In the method of collective behavior the passage from classical to quantum type of consideration means simply the change of swarm size, e.g. does not mean the different type of dynamics. Due to the above mentioned reserve in the choice of resolution in the process of film preparation we then can further decrease the values δx and δt for the forming of right picture , for example, dividing these intervals to smaller parts and obtain the better approximation to the solution of Shredinger equation. We assume that the space R^3 is divided to the equal cubes with the side δx, and the time is divided to the equal intervals of the longitude δt.

We introduce the value c, which is the single nonzero speed of movement of the samples in the swarm. The intervals of time and distances will be always chosen so that $\delta x \gg c\delta t$. It guarantees that in each step of the evolution the values of magnitudes obtained as the mean values on cubes with the side δx will change small that is necessary for the asymptotical approximation.

The density of swarm in the point x is determined by the expression

$$\rho(r,t) = \frac{N(r,t)}{(\delta x)^3}, \tag{3.1}$$

where $N(r,t)$ denotes the total number of samples occurring in the moment t in the same cube with the point r. For the comparison with Shredinger equation in this definition we should converge $\delta x \longrightarrow 0$, that means the consideration of the sequence of the swarms with the densities ρ_n with the growing n instead of one swarm. Further we assume that the value δx is fixed. We write $\rho(x) = |\Psi(x)|^2$ instead of

$$\rho_n(x) \longrightarrow |\Psi(x)|^2 (n \longrightarrow \infty), \tag{3.2}$$

where the convergence is uniform without special mentioning. This sequence of the swarms realizing the approximation of the exact solution of Shredinger equation is called the admissible approximation of quantum evolution.

Our aim is to define the behavior of the samples in the swarm which gives the admissible approximation of quantum evolution.

The main requirements to the simulation of quantum dynamics through the collective behavior are the following.

- Quantum dynamics is simulated by the dynamics of the swarm of samples so that in each time instant t the quantum probability equals the density of the swarm.

$$|\Psi(x,t)|^2 = \rho(x,t) \qquad (3.3)$$

  in each point x of the configuration space.

- Each sample of the swarm has its own history, e.g. it preserves its individual number in course of the whole simulating process. The types of the samples exactly correspond to the types of real physical particles.

- The behavior of each sample is completely determined by its own state and the state of all samples in its close vicinity.

The swarm satisfying these conditions is called the quantum swarm for one quantum particle.

We define the behavior of the samples such that these conditions are satisfied. For this it is sufficient to show that for the solution $\Psi(x,t)$ of Shredinger equation it is possible to move the samples only locally, e.g. to the small distance for the insurance of the equation (3.3) in each time instant. Such a movement, of course, will be a priori non natural in the dynamical sense, but we will show how it can be done by means of the dynamical diffusion mechanism.

We note that the second rule means that we refuse from the using of complex numbers in the description of quantum mechanics. Also the locality of all interactions allows including QED to our model. The behavior of samples is the rule determining the change of its internal states (the type, impulse, momentum of impulse) and the spatial position (spatial shift). In view of the above mentioned the behavior cannot be determined by the classical physics.

We define the quasi classical behavior of the samples called the dynamical diffusion mechanism. The swarm of samples with such behavior satisfies these conditions.

Let us agree that each sample in each time instant can either to stay in place or to move along one of the coordinate axes OX, OY, OZ with the speed c.

We call the reaction of change the sequence of the following operations on the swarm: the choice of pair α, β of the samples located not farer than δx from each other, which speeds are mutually opposite: $v(\alpha) = -v(\beta)$ and either simultaneous replacement of their speeds to zero (if they are nonzero) or acquiring them mutually opposite speeds of the module c oriented along one of the coordinate axe. The axe is always chosen randomly from the uniform probability distribution.

The reaction of change does not change neither summed impulse of the swarm, nor summed momentum of impulse if δx is sufficiently small. By $N(r)$ and $N_s(r)$ we denote the sets of all samples in the cube with the point r and the set of samples from this cube possessing zero speeds correspondingly; by $N^+{}_x(r), N^+{}_y(r), N^+{}_z(r)$

we denote the sets of samples from the cube r, moving along the corresponding axe in the positive direction, and by analogous symbols with the sign $-$ the corresponding sets but for the negative direction of movement. By $|g|$ we denote the total number of samples in the set g. Let us agree to denote the total numbers of samples in a set by the same symbol as this set but with the replacement N to n. We call r-stationary each subset $S \subseteq n(r)$ consisting of the samples with nonzero speeds for which $\sum_{\alpha \in S} v(\alpha) = 0$ and S is the maximal on including with this property. The total number $|S|$ of the samples of r-stationary set (which does not depend on its choice) is denoted by $s(r)$. Let $d > 0$ be a chosen constant such that the coefficient of the diffusion is proportional to d, $V(r)$ is a scalar field proportional to the external potential energy with the constant coefficient of proportionality, $grad\,V(r) = $ $= (V_x(r), V_y(r), V_z(r))$.

We also agree to consider only non relativistic swarms, e.g. such that $n_s(r)/n(r)$ is close to 1 for all r. It means that the bulk of samples in each cube have zero speed. This requirement is incompatible with the point wise approximation by the swarms 3.2 of the exact wave functions for the external potential of Coulomb form $1/r$ because the mean speed of samples in the vicinity of zero point for such potentials must converge to infinity. For the asymptotic convergence 3.2 we would have to assume that c can be chosen as large as needed for every next swarm number n. In the reality c cannot exceed the speed of light that establishes the natural limitation to the accuracy of the swarm approximation of the solutions of Shredinger equation.

The dynamical diffusion mechanism of evolution is the following sequence of the operation on the swarm:

- 1) The sequence of random reactions of change with the uniform distribution of probability, which gives the distribution of the speeds with the property $s(r)/n_s(r) = d$ for each point r. If $n(r)$ is small, this equality must be satisfied with the maximal accuracy (see agreement about the accuracy from above).

- 2) The acquiring of speeds to some samples from $N_s(r)$, randomly chosen from the uniform distribution so that for each axe the signs of newly acquired speeds along this axe are the same, and if $v_u(r)$ is the summed speed acquired to the samples from r-th cube along the axe u, $u = x, y, z$, then for all such u the equation $v_u(r)m = -V_u(r)$ is fulfilled with the maximal possible accuracy.

- 3) The change of coordinates $r(\alpha)$ of each sample corresponding to the Galileo law: $r_{new}(\alpha) = r(\alpha) + v(\alpha)\Delta t$.

- 4) Recalculation of $V(r)$ accordingly to the new positions of samples.

We do not concretize the method of recalculation of the potential energy. It may be done by Coulomb formula or by the diffusion mechanism as was proposed in the work [**?**].

The dynamical diffusion swarm cannot be represented as an ensemble of point wise particles with the classical interaction. The item 1) says about two things:

- there is the force with the random direction which acts to the samples (compare with [**?**]), and

- the samples acquire the mean value of speed within the accuracy determined by δx (the lesser δx is the more accurate mean value is taken).

For each time instant t if Δx is sufficiently small then the density of swarm $\rho(r, t)$ for any point r will not depend on the orientation of the coordinate axes. Indeed, let δ_1 be such that $c\delta t \ll \delta_1 x \ll \delta x$, and let $v(r)$ denote the average speed of the samples in the point r, found by the averaging on the samples with the coordinates $r_1 : \|r - r_1\| < \delta_1 x$. The total number of the samples occurred in the unit of time from the vicinity of the point r_1 to the vicinity of the close point r_2 will be then proportional to the dot product $v(r_1)(r_2 - r_1)/\|r_2 - r_1\|^2$, which does not depend on the orientation of the coordinate axes.

A state of the dynamical diffusion swarm is determined by the coordinates and speeds of all its samples. This is its principal difference from the ensemble of DMC method where there are no speeds of the samples.

4. Differential equations for the dynamical diffusion swarm

There is no system of differential equations on the density of the diffusion swarm and its average speed which is equivalent to Shredinger equation.

Nevertheless, there is the sequence of such systems which realizes the admissible asymptotic approximation of the solution of Shredinger equation. Each of the system from this sequence depends on the fixed elementary length δx. For example, the intensiveness of the diffusion process will beb proportional to $(\delta x)^{-3}$. This does not allow to launch δx to zero as it is always done in the mathematical analysis when it is applied to the processes of classical physics. The value of grain δx must be chosen such that the approximation of the density $\rho = |\Psi|^2$ of the wave function by the density of the diffusion swarm within $(\delta x)^3$ is satisfactory for the considered process. Only after the fixation of δx it is possible to build the diffusion swarm of the corresponding intensiveness and the differential equations approximating its dynamics which will be equivalent to Shredinger equation.

A state of the dynamical diffusion swarm is determined by the pair of functions

$$\rho(t, \bar{r}), \ \bar{p}(t, \bar{r}), \tag{4.1}$$

where ρ is the scalar function of density of the samples, $\bar{p}(\bar{r})$ is the vector function resulting impulse of the samples in the point $\bar{r}$ defined as $\lim\limits_{dx \longrightarrow 0} P(r, dx)/(dx)^3$, where P is the summed impulse of the samples occurred in the cube with r with the side dx. Here we assumed that dx can be done sufficiently less than the grain δx, determining the coefficients of the equation on ρ and $\bar{p}$.

The dependence of equations on the grain δx will be revealed as follows. The summed impulse $\bar{p}(t, \bar{r})$ varies slowly when $\bar{r}$ changes on values larger than δx. But its derivative $\dfrac{\partial \bar{p}}{\partial t}$ will be very large: of the order $1/(\delta x)^3$, and will vary rapidly as well. E.g., the graph of the function $\bar{p}(t, \bar{r})$ is sufficiently smooth if we look at it with the large grain δx, but if we raise the resolution by decreasing the grain δx, we see that the graph looks like a saw with acute teeth. The more is resolution $1/\delta x$ the

more is sharpening of the teeth, it is limited by the limit of speed c (compare with [**?**]). This important for further condition we call the non relativistic approximation and will write it as $v \ll c$.

In view of isotropy of the diffusion process the change of density $\rho(r,t)$ in the time and its second derivative can be found by the integration on the surface of the sphere $S(r)$ of radius δx by formulas

$$
\begin{aligned}
\frac{\partial \rho(r,t)}{\partial t} &= \int\limits_{S(r)} \bar{p}(r,t)\bar{n}(\bar{r}_1)ds(r_1), \\
\frac{\partial^2 \rho(r,t)}{\partial t^2} &= \int\limits_{S(r)} \frac{\partial \bar{p}(r,t)}{\partial t}\bar{n}(\bar{r}_1)ds(r_1).
\end{aligned}
\tag{4.2}
$$

These formulas are right for any mechanism of changing of the speed of samples.

Now we derive the law of changing of the resulting impulse $\frac{\partial \bar{p}}{\partial t}\bar{a}$ of the swarm in the small sphere with center in the point $\bar{r}$, which results from the moveme of the samples along the vector $\bar{a}$ of normal to the surface of sphere of the unit length. Three magnitudes make the deposits to the change of the resulting impulse:

- Penetration of the samples which have acquired the speed in the reaction of change through the small element of the surface (diffusion).

- Penetration of the samples which have acquired the speed from the action of external potential.

- Penetration of the samples which have preserved their speed (by inertia).

It follows from the definition of the diffusion process that these deposits equal correspondingly $-I \operatorname{grad} \rho \bar{a}$, $-\kappa\rho \operatorname{grad} V \bar{a}$ and $g\rho\bar{p}\bar{a}$, where I, κ, g is the intensities of the corresponding processes. The choice of units system allows us to make $g = 1$. The dependence of the grain of spatial resolution needed for approximation of Shredinger equation has the form:

$$
I = \frac{h^2}{2m^2(\delta x)^3}, \ \kappa = \frac{h}{m\delta x}.
\tag{4.3}
$$

In view of the non relativistic supposition we can omit the last summand which is sufficiently smaller than the first two for the small δx. We then obtain the following approximate formula.

$$
\frac{\partial \bar{p}}{\partial t} \approx -I \operatorname{grad} \rho - \kappa\rho \operatorname{grad} V.
\tag{4.4}
$$

The resulting equation on the density of the diffusion swarm has thus the form:

$$
\frac{\partial^2 \rho(r)}{\partial t^2} = -\int\limits_{S(r)} I \operatorname{grad} \rho - \kappa\rho \operatorname{grad} V)\bar{n}(r') \, dS(r'),
\tag{4.5}
$$

where the coefficients I, κ can be found by 4.3.

We prove that the quantum swarm satisfies 4.5, which means the admissible approximation of the quantum dynamics by the evolution of the swarm.

The method of collective behavior permits to give the simple algorithm for the computation of the energy, impulse and momentum of impulse of quantum particle represented as the swarm of samples. Here accordingly to the quantum rules for the finding of any magnitude we have to averaging on the values of the reciprocal magnitude. To find the impulse we must fix some value of the time interval Δt and fulfill averaging of impulses on all samples on any values of the distances they overcome. This receipt in our notations gives the vector

$$(\sum_r cm\frac{n_x(r)^+ - n_x(r)^-}{n(r)}, cm\frac{n_y(r)^+ - n_y(r)^-}{n(r)}, cm\frac{n_z(r)^+ - n_z(r)^-}{n(r)}) \qquad (4.6)$$

which equals to the average impulse of all samples in the swarm found by averaging on the passes in the fixed time interval. The analogous calculation of the momentum of impulse or the potential energy gives the average momentum or the average potential energy.

When calculating the average kinetic energy we have to fix the pass δx and to take the average energy on all instant of the time t, because the time is the reciprocal magnitude for the energy. It means that we must sum only the energies of the samples which are moving in the considered time instant, e.g., for any cube for the speed $v = = cn_x/n$ along the axe x the expected total number of such samples is nv/c, and their fraction in the total number of samples is n_x/n. Here we use the non relativistic assumption that the total fraction of the moving samples is small. The total kinetic energy found by this rule is

$$mc^2 n_x n_x/n + mc^2 n_y n_y/n + mc^2 n_z n_z/n$$

which coincides to the kinetic energy found by the conventional formula $Mv^2_{mean}/2 = = ((cn_x/n)^2 + (cn_y/n)^2 + (cn_z/n)^2)nm/2$. The laws of conservations for the impulse, momentum of impulse, energy of the swarm then follow from the classical laws of conservation and the non relativistic assumption. In the next paragraph we prove that the diffusion swarm dynamics can give the admissible approximation of the quantum one. Using Erenfest theorems and the laws of conservation for quantum dynamics we conclude that our method of calculation of these magnitudes A gives their quantum mean values found by the formula $\langle A \rangle = \int \Psi^*(r)A\Psi(r)dr$.

5. About the diffusion swarm with non uniform intensity

The intensiveness of the diffusion equals the coefficient of the Laplace operator in the diffusion equation. The intensiveness determines the total number of samples passing through the unit of square in the unit of time. To simulate quantum dynamics we need the diffusion swarm with the non uniform intensiveness. It means that the intensiveness of diffusion depends on the chosen grain of the spatial resolution δx. In this section we discuss how non uniform intensiveness of diffusion can be obtained

in the same swarm. The concrete mechanisms discussed here will not be used further; they can be interesting only for the programming realization of the dynamical diffusion method.

We at first consider the case when the external potential is constant $grad\, V = 0$. The dynamical diffusion process with the non uniform intensiveness can be insured by the special mechanism which we call threads. We illustrate the method on the following example. We suppose that all samples move not in all the space but along one closed trajectory (thread) which is determined by the smooth embedment of the circle to the space: $\gamma : \ S^1 \longrightarrow R^3$. We suppose that the change of speeds happens only along this trajectory so that the samples remain in this thread in each time instant. This is equivalent to the imposing of the holonomic tie to the samples. We then suppose that the linear density as well as the module of speed of the samples is almost equal in all point of the trajectory. We consider the cube containing one point of this trajectory. The flow of samples through its border will not depend on its size δx, because the thread is only one. The intensiveness of this process is thus proportional $1/(\delta x)^3$, because the quantity of samples penetrating in unit of time into the cube with the side δx does not depend on δx, and the density is obtained by the division of the quantity of samples to the volume. This example is not very good because many areas of the space remain without the samples at all.

We consider the next example. Let the space be divided to the cubes which are grouped by the layers $1, 2, \ldots$. For each $j = 1, 2, \ldots$ the cubes of the layer $j + 1$ consist of 8 cubes of the layer j, and their side, correspondingly, is twice large. For each j the change of samples between the neighbor cubes of the layer j, occurring to the same cube of the layer $j + 1$, goes only through the narrow channel with small capacity independent of j. The quantity of samples moving between the cubes of any fixed layer will not then depend on the number of this layer. It can be guaranteed by the appropriate choice of the pair for the change of impulses. Such a mechanism gives us the required intensiveness of the diffusion proportional to $1/(\delta x)^3$, in view of the definition of density (8.4).

Now we consider the case of varying external potential. At each step of the evolution for the samples acquiring or loosing their speeds in the change we will use the rule from above, which insures the intensiveness proportional to $1/(\delta x)^3$. The samples acquiring their speed from the action of the external potential will move as usual, independently of layers. We then obtain the formula (4.3). This space design show how in principle the necessary non uniform intensiveness can be obtained in on swarm.

Practical realization of these methods presumes that we trace for the spatial location of the separated parts of the swarm, which means the refusal from the uniformity of the space and passage to the fractal space. The space with fractal dimensionality arises if we use the non uniform grid for the method of finite elements. This is why the proposed computational receipt says that we must fix the grain δx of the linear resolution such that the corresponding approximation of the wave function is satisfactory for our aims, and then consider the diffusion swarm with the intensiveness found by 4.3. If we are not satisfied with the obtained dynamical picture, we must choose the new value of δx and repeat all the work.

6. Equivalence of quantum and dynamical diffusion swarms

Here we show that the sequence of diffusion swarms represents the admissible approximation of quantum evolution. We have defined the quantum swarm as the swarm satisfying 3.3 and which evolution can be represented as the local movements of the samples.

At first we determine that the quantum swarm exists, e.g., that the equation 3.3 can be really reached by only local shifts of the samples. Then we prove that the mechanism of the movements of samples coincides with the diffusion that gives the main result.

Let us consider the quantum swarm. We start with Shredinger equation

$$ih\frac{\partial \Psi(r,t)}{\partial t} = -\frac{h^2}{2M}\Delta\Psi(r,t) + V_{pot}(r,t)\Psi(r,t), \tag{6.1}$$

which can be rewritten as

$$\begin{aligned}
\Psi_t^r(r) &= -\frac{h}{2M}\Delta\Psi_t^i(r) + \frac{V_{pot}}{h}\Psi^i(r), \\
\Psi_t^i(r) &= \frac{h}{2M}\Delta\Psi_t^r(r) - \frac{V_{pot}}{h}\Psi^r(r)
\end{aligned} \tag{6.2}$$

for the real and imaginary parts Ψ^r, Ψ^i of the wave function Ψ. We focus on the evolution of the density of quantum swarm, which is the function

$$\rho(r,t) = (\Psi^r(r,t))^2 + (\Psi^i(r,t))^2.$$

Fixing the value of δx we apply for the approximation of the second derivative the difference scheme of the form

$$\frac{\partial^2 \Psi(x)}{\partial x^2} \approx \frac{\Psi(x+\delta x) + \Psi(x-\delta x) - 2\Psi(x)}{(\delta x)^2}$$

for each time instant, where the wave function is supposed to satisfy all the sufficient conditions for such approximation. Since the addition of any constant to the potential energy V_{pot} does not influence to the quantum evolution of the density, we can consider instead of V_{pot} the other potential $V = V_{pot} + \alpha$, where $\alpha = -\frac{3h^2}{m(\delta x)^2}$, that leads to the disappearing of the summand $2\Psi(x)$ in the difference schemes for the second derivative on x, y, z (from which the coefficient 3 arises) after its substitution to Shredinger equation. We introduce the simplifying coefficient

$$\gamma = \frac{h}{2M}\frac{1}{(\delta x)^2}.$$

Since we yet do not know the mechanism of moving of the samples in quantum swarm, we suppose that we simply either take off some quantity of the samples from any cube or put it there from some storage. We split the evolution of the quantum

swarm in the time to so small segments of the longitude δt, that in each of which the samples move only in the framework of two neighbor cubes. If we prove that the evolution of quantum swarm on such segment is insured by the diffusion mechanism, it will be right for the whole evolution as well. That is our supposition does not limit the generality. We also agree that these cubes differ from one another by the shift to δx along the axe x, that does not limit the generality as well. Let the centers of these cubes be x and $x_1 = x + \delta x$. In these suppositions the summand $\Psi(x - \delta x)$ in the difference scheme disappears as well and on the considered small time segment the evolution of quantum swarm is determined by the system of equations:

$$
\begin{aligned}
\Psi_t^r(x) &= -\gamma \Psi^i(x_1) + V(x)\Psi^i(x), \\
\Psi_t^i(x) &= \gamma \Psi^r(x_1) - V(x)\Psi^r(x),
\end{aligned}
\tag{6.3}
$$

and by the analogous system obtained by the substitution of x in place of x_1 and vise versa.

For such a segment we thus have

$$
\begin{aligned}
\frac{\partial \rho(x)}{\partial t} &= 2\Psi^i(x)(\gamma \Psi^r(x_1) - V(x)\Psi^r(x)) \quad +2\Psi^r(x)(-\gamma \Psi^i(x_1) - V(x)\Psi^i(x)) = \\
&= 2\gamma(\Psi^i(x)\Psi^r(x_1) - \Psi^r(x)\Psi^i(x_1)) \quad = -\frac{\partial \rho(x_1)}{\partial t}.
\end{aligned}
\tag{6.4}
$$

It results in that the outcome of the samples in one cube equals their income to the other. The evolution of quantum swarm then satisfies the condition of locality. In the order to compare these evolution with the diffusion we now find the second derivative of the quantum density to time:

$$
\begin{aligned}
\frac{\partial^2 \rho(x)}{\partial t^2} &= 2\gamma[(\gamma \Psi^r(x_1) - V(x)\Psi^r(x))\Psi^r(x_1) + \Psi^i(x)(-\gamma \Psi^i(x) + V(x_1)\Psi^i(x_1)) - \\
&(-\gamma \Psi^i(x_1) + V(x)\Psi^i(x))\Psi^i(x_1) - \Psi^r(x)(\gamma \Psi^r(x) - V(x_1)\Psi^r(x_1))] = \\
&2\gamma^2(\Psi^r(x_1))^2 - 2\gamma V(x)\Psi^r(x)\Psi^r(x_1) - 2\gamma^2(\Psi^i(x))^2 + \\
&2\gamma V(x_1)\Psi^i(x)\Psi^i(x_1) + 2\gamma^2(\Psi^i(x_1))^2 - 2\gamma V(x)\Psi^i(x)\Psi^i(x_1) - \\
&2\gamma^2(\Psi^r(x))^2 + 2\gamma V(x_1)\Psi^r(x)\Psi^r(x_1) = \\
&2\gamma^2((\Psi^r(x_1))^2 + (\Psi^i(x_1))^2 - ((\Psi^r(x))^2 + (\Psi^i(x))^2)) + \\
&2\gamma[(V(x_1) - V(x))((\Psi^r(x))^2 + (\Psi^i(x))^2) + o(\delta x)],
\end{aligned}
\tag{6.5}
$$

where $o(\delta x) = (\Psi^r(x)\Psi^r(x_1) + \Psi^i(x)\Psi^i(x_1) - ((\Psi^r(x))^2 + (\Psi^i(x))^2))(V(x_1) - V(x))$. Now we compare it with the expression for the second derivative of the density of diffusion swarm found in the previous section, taking into account that in our case the change of samples goes between two neighbor cubes along the axe x only. Comparing with 4.5 in view of 4.3, we conclude that the second derivative of the density of quantum swarm asymptotically converge to the second derivative of diffusion swarm.

If we choose instead of the initial state the state where its density has Gauss form which is the ground state of harmonic oscillator, then for the corresponding value of energy $V = a(x^2 + y^2 + z^2)$ we have $\partial \rho / \partial t = 0$ in the initial instant for any point of space. It is proved that the second derivative of the quantum swarm density and of the diffusion swarm density are the same, hence the diffusion swarm will be

good approximation for the quantum density on some interval ΔT. Switching on slowly some potential we will have also the approximation of any quantum evolution in the limit of swarms for the unlimited increasing of n.

The swarm approximating quantum dynamics of one particle depends on the choice of δx. After the fixation of δx we obtain for unlimitedly decreasing δt the approximation of the wave function within δx. The intensiveness of the diffusion will be determined by δx, it will be $\dfrac{h^3}{m^3 c(\delta x)^3}$. If we want to decrease the grain δx we must allow the more quantity of moving samples in the unit volume. It is necessary due to the uncertainty principle for length and impulse: the dispersion of speeds of the samples will grow if δx decreases. In any case for the obtaining of the dynamical picture one has to fix the grain of spatial resolution δx.

If the total number of samples n is limited we obtain the model of quantum dynamics with decoherence of the inbuilt type. This model can be extended to the multi particle case where it can serve as the approximation of quantum dynamics in the standard Hilbert formalism (see ([**?**]). The robustness of this scheme for the numerical computations follows from that it gives Born rule for the quantum probability which thus turns to be inbuilt into the algorithmic formalism, in contrast to Copenhagen formalism where this rule is postulated.

7. Restoration of wave function from dynamical diffusion swarm

We have solved the problem of approximation of the dynamics of density for one quantum particle by the special diffusion process with the non uniform intensity. A state of the dynamical diffusion swarm is determined by a pair 4.1. Such a pair does not contain the notion of complex numbers which induced the famous quantum interference in the standard formalism. Furthermore, the diffusion swarm gives no beautiful differential equations of Shredinger type for ρ and $\bar{p}$. It radically differs from the classical processes (for example, heat transform or oscillations) because its intensity depends on the chosen grain of spatial resolution. We agree to these for the sake of the main: the economy of the computational resources required for the description of quantum dynamics.

Now, to finalize the picture we have to solve the inverse problem: to show how to restore the wave function Ψ from the given state of the dynamical diffusion swarm 4.1. to do this we turn to the equality 6.4, and substitute to it the expression of the wave function through the density: $\Psi(r) = \sqrt{\rho(r)} \exp(i\phi(r))$. We must find the phase $\phi(r)$ of the wave function. Since only relative phase has the physical sense we can fix some point r and consider the phase of the other point r_1 relatively to r. If r_1 is close to r, the equation 6.4 gives us

$$\phi(r) - \phi(r_1) = arcsin\ k(\delta x)^2 \frac{\bar{p}(\bar{r} - \bar{r}_1)}{\sqrt{\rho(r)\rho(r_1)}}$$

which results in the following formula for the finding of the relative phase:

$$\phi(r_1) = \int\limits_{\gamma} k(\delta x)^2 \bar{v} \; d\bar{\gamma} \qquad (7.1)$$

where the contour γ goes from r to r_1. This definition depends explicitly on the choice of contour γ, hence we have to prove its correctness, e.g., its independence of the contour γ. Since the phase is determined within an integer multiplier of 2π, the different choices of the contour can result at most in the change of the phase on such a number that takes place in case of excited states of electron in hydrogen atom with the nonzero momentum (for example, $3d$). We show that the integration of speed $\bar{v}$ of the swarm on the closed contour preserves its value in the time with the more exactness the less δx is. It involves that if in the initial time instant the definition (7.1) was correct, it then remains correct for the next time instants.

We now consider the derivative of the integral of the speed for the closed contour γ_c. Applying the formula (4.5) and accounting $\partial \bar{p}/\partial t = \rho \; \partial \bar{v}/\partial t$, we obtain

$$\frac{\partial}{\partial t} \int\limits_{\gamma_c} (\delta x)^2 \bar{v} \; d\gamma = - \int\limits_{\gamma_c} I(\delta x)^2 \frac{grad \; \rho}{\rho} + \kappa (\delta x)^2 \; grad \; V. \qquad (7.2)$$

The first summand gives zero after the integration on the closed contour, because it is $grad \; \ln \rho$, the second summand gives zero by analogous reason.

Now it is sufficient to verify the correctness of the definition (7.1) in the initial time instant that can be done immediately for any task. If the wave function of initial state can be obtained from the ground state in the Coulomb field where $\bar{v} = 0$, then the correctness follows from the proved because there is no any phase shift here to $2\pi k$. If for the obtaining of the initial state in the considered problem we must start from some excited state with the shift of the phase, the correctness should be checked for this state at first.

8. Collective behavior for n particles

Let we are given a set of n quantum particles that we enumerate by integers: $1, 2, \ldots, n$. We assume that the main act of evolution is the reaction of scattering when these particles fly to each other simultaneously and can associate in some stable complex objects called molecules. Factually, the more general picture of scattering takes place: initial particles can consist of some more elementary particles, and in the reaction these more elementary particles can regroup and form the products of the reactions, which consist of the same elementary particles as the initial objects, but in the other configurations.

The simple example of such a reaction is the scattering of a proton on an atom of hydrogen. Here the moving proton (proton number one) flies to the staying hydrogen atom which in turn consists of an electron and proton number two. The possible products are: a) isolated proton number one and hydrogen atom, b) isolated proton number two and hydrogen atom formed by the electron and the proton number one

(the recharge), c) forming of the molecular ion of hydrogen (two protons glued by the electron), and d) separate protons and electrons. The cases b) and c) represent the main interest here because we then have the recombination of constituents (b) or association of the new molecule (c).

We assume that the right description of the elementary reactions with n particles is sufficient to build the actual model of the processes of any degree of complexity including the description of the simple forms of living entities, like viruses and bacteria. Namely, the easy generalization of abstract methods for scattering will give us the picture of the behavior of very complex objects.

The main requirement to these types of models is that the required time and memory for the simulation must grow not faster than linearly of the total number n of participating particles, and the single essentially not conventional procedure in the simulation is the simulation of decoherence.

The easiest algorithmic model of decoherence is called the absolute decoherence model. It claims that decoherence comes as the reduction of quantum state

$$|\Psi\rangle = \sum_j \lambda_j |j\rangle \tag{8.1}$$

in the instant when the memory of the simulating computer cannot include the whole notation of this state. The absolute model can be concretized as follows. We suppose that the amplitudes in 8.1 cannot exceed some level $\epsilon > 0$, called amplitude grain. If in the unitary evolution some amplitude λ_j becomes less than ϵ, the corresponding summand $\lambda_j |j\rangle$ is merely excluded from the state 8.1, with the corresponding renormalization of state. In the work [3] it was shown that this simple rule gives the Born rule for probability to obtain the state $|j\rangle$ as the result of measurement of $\|psi\rangle$ as $p_j = |\lambda_j|^2$. But this is yet not the final form of simulating algorithm because the rule of small amplitude reduction requires matrix algebra technique and thus cannot serve as the core of simulating algorithms due to the non economical essence of matrix computations.

To obtain the robust scheme of simulating algorithm we must sequentially use the method of collective behavior, where the algorithmic reduction of quantum state is the inbuilt property. Let us consider the swarm representation of our n particles $1, 2, \ldots, n$, where $S_1, S_2, \ldots, S_n$ are the swarms of samples corresponding to their states $|\Psi_1\rangle, |\Psi_2\rangle, \ldots, |\Psi_n\rangle$. If we consider the ensemble consisting of all these samples, it will be the representation of non entangled state of the form $|\Psi_1\rangle \bigotimes |\Psi_2\rangle \bigotimes \ldots \bigotimes |\Psi_n\rangle$. But to represent the entangled state of the form

$$\Phi\rangle = \sum_{j_1, j_2, \ldots, j_n} \lambda_{j_1, j_2, \ldots, j_n} |j_1, j_2, \ldots, j_n\rangle \tag{8.2}$$

we must introduce the new and crucial element to the method of collective behavior. This is the bonds between the samples of the different swarms. The basic state j_i can be treated as the coordinate of particle i in the corresponding configuration space. The representation of wave function in the form 8.2 means that there are bonds connecting points $j_1, j_2, \ldots, j_n$ in one cortege. The relative quantity of bonds of this form (their total number divided to the total number of all bonds) is $|\lambda_{j_1, j_2, \ldots, j_n}|^2$.

We assume that the bonds connect not spatial points but the samples of real particles. They have the form of corteges

$$\bar{s} = (s_1, s_2, \ldots, s_n) \tag{8.3}$$

where for any $j = 1, 2, \ldots, n$ $s_j \in S_j$. The wave function $|\Phi\rangle$ is then represented by the set $\bar{S}$ of corteges $\bar{s}$ so that for each $j = 1, 2, \ldots,$ $s_j \in S_j$ there exist exactly one cortege of the form 8.3. Each cortege plays the role of the so called world in the many world interpretation of quantum theory. We treat this cortege 8.3 as one probe representation of the n particle system and all interactions goes inside the same cortege whereas the real system state results from the interference of amplitudes corresponding to all cortege which occur in the same spatial cell. We call $\bar{S}$ the swarm for n particle system.

The density of the swarm $\bar{S}$ is defined as

$$\rho_{\bar{S}}(r_1, r_2, \ldots, r_n) = \lim_{dx \longrightarrow \infty} \frac{N_{r_1, r_2, \ldots, r_n, \, dx}}{(dx)^{3n}}, \tag{8.4}$$

where $N_{r_1, r_2, \ldots, r_n, \, dx}$ is the total number of cortege which occur in the $3n$ dimensional cube with the side dx and the center $r_1, r_2, \ldots, r_n$.

If the wave function $|\Phi\rangle$ is the tensor product of one particle wave functions:

$$\Phi\rangle = \bigotimes_{i=1}^{n} |\phi_i\rangle$$

The corresponding bonds can be obtained by random choice of samples $s_j \in S_j$ for each $j = 1, 2, \ldots, n$, forming one cortege $s_1, s_2, \ldots, s_n$. With this choice of cortege we obtain that the density of swarm satisfy the Born condition which can be written for swarms in the form

$$\sum_{\bar{r} \in D} |\langle \bar{r} | \Phi \rangle|^2 = \frac{N_{\bar{r}, \bar{S}}}{N} \tag{8.5}$$

where $D \subset R^{3n}$, $N_{\bar{r}, \bar{S}}$ is the total number of corteges occur in the area D. But for the entangled state $|\Phi\rangle$ this choice of corteges for the kit $\bar{S}$ will not give us the equality 8.5. We thus must take 8.5 as the definition of the choice of corteges in $\bar{S}$. But to define the swarm we also need the velocities for all samples, namely, we need the generalization of rules from the previous paragraph to the case of n real quantum particles.

Let $\Psi(r_1, r_2, \ldots, r_n)$ be the wave function of n particle system, $\Psi = = |\Psi| exp(i\phi(r_1, r_2, \ldots, r_n)$ be its Euler expansion. We denote by $\mathrm{grad}_j \, \phi(r_1, r_2, \ldots, r_n)$ the gradient of Ψ taken on the coordinates of particle j, where $j \in \{1, 2, \ldots, n\}$ is the fixed integer. The generalization of formulas from the previous paragraph to the n particle case has the form

$$\begin{aligned} &|\Psi(\bar{r})| = \sqrt{\rho(\bar{r})}; \\ &\phi(r) = \int_{\bar{\gamma}: \, \bar{r}_0 \longrightarrow \bar{r}} k(dx)^2 \bar{v} \cdot d\gamma, \\ &\bar{v} = a(dx)^{-2} \mathrm{grad} \, \phi(\bar{r}), \end{aligned} \tag{8.6}$$

where $\bar{r}$ means $r_1, r_2, \ldots, r_n$, $\bar{\text{grad}}$ means $\text{grad}_1, \text{grad}_2, \ldots, \text{grad}_n$, and $\bar{\gamma}$ is the path in $3n$ dimensional space. The rules 8.6 is sufficient to determine the swarm given the wave function, if we agree to join the samples into corteges independently of their velocities. The microscopic mechanism of swarm dynamics takes the following form. Impulse exchange between two corteges of samples: $\bar{s} = (s_1, s_2, \ldots, s_j, \ldots, s_n)$ and $\bar{s} = (s_1, s_2, \ldots, s_j, \ldots, s_n)$ is impulse exchange between the two samples s_j and s_j provided $\bar{s}$ and $\bar{s}$ belong to the same spatial cube in the configuration space R^{3n} for n particles. With this definition the reasoning from the paper [12] can be repeated straightforwardly and we obtain that this microscopic mechanism of impulse exchange for n particles ensures the approximation of n particle quantum dynamics within the accuracy of the order dx^{3n} in the determining of wave function.

The described method of collective behavior gives us the good framework for the economical simulation of quantum evolution.

9. Genetic method of entangling

The method of collective behavior yet does not give us the algorithm for simulation of quantum system dynamics, because the starting point of this method requires the wave function description. To make the collective behavior method complete we must point how to perform entangling, that is how to choose the initial corteges of samples. This choice must guarantee the best approximation of wave function by corteges 8.6. We then can treat one sample as a currier of amplitude grain in sense of [3], and the swarm dynamics will thus give us the approximation of unitary dynamics and decoherence simultaneously. The task of choosing corteges is thus the core of quantum simulation.

The experiments in the real simulation show that the task of choice of corteges can hardly be solved by the one step procedure. I suggest the following simple genetic algorithm for finding the corteges, which uses the sequential repetitions of dynamical scenarios when the choice of initial conditions for each repetition will use the result of the previous one.

We will describe the genetic entangling on the example of scattering of n quantum particles. We start from the non entangled state of them where the particle j state is determined by the wave function Ψ_j, or, in swarm representation, by the swarm S_j. At the first scenario to determine the initial state of our swarm $\bar{S}_{ini}$ we choose the corteges $\bar{s}$ at random. After the fixed small time of evolution Δt of the swarm we obtain its final state $\bar{S}_{fin}$. If we have a huge total number N of samples beforehand, in the swarms S_j, we would obtain the good approximation of wave function by $\bar{S}_{fin}$, where the final quantity of all samples will serve as the decoherence factor. The problem is to use the strictly limited number N of the samples to simulate the real dynamics with the admissible accuracy. Here in case of scattering under admissible accuracy we mean the right separation of the products of reactions: for chemical reactions there is the list of possible products with the corresponding probabilities depending on the initial state of reagents. With this limitation of N we must charge the samples with the two roles: the first is to simulate the unitary dynamics of the wave function, and the second is to simulate the decoherence result-

ing from the amplitude grain. We note that these two role are not in full agreement with each other. The approximation of the wave function requires the small distance $\|\Psi_{Shoedinger} - \Psi_{swarm}\|$ whereas the decoherence resulting from the amplitude grain nulls all states with the amplitude module less than ϵ that can give the big discrepancy with the wave function in the unitary evolution especially when the dispersion of amplitude distribution is large.

We thus have to choose corteges $\bar{s}$ so that the distribution of samples among them be the most economical for unitary dynamics as well as for decoherence on the short time segment Δt. Call the space R^{6n} double configuration space for n particles. The sense of it is that we will consider the pair of states: initial and final. For each cortege $\bar{s}_{ini}$ in the initial swarm there is one and only one cortege $\bar{s}_{fin}$ which results from $\bar{s}_{ini}$ in the swarm evolution. We choose the division of double configuration space for n particles to the cells of the form of cubes, and group the resulting pairs $(\bar{s}_{ini}, \bar{s}_{fin})$ of corteges into groups $\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_k$ so that each group consists of all pairs which occur in the same spatial cube of the division. Let the numbers of elements $\mathcal{N}_j$ in these groups be ordered directly: $\mathcal{N}_1 \geq \mathcal{N}_2 \geq \ldots \geq \mathcal{N}_k$. We choose the first $k_1 < k$ groups and call the pairs in them right pairs. The other pairs are called wrong. We are now ready to obtain the initial state for the next repetition of scattering. We exclude the wrong pairs from $\bar{S}$ and reorganize their members to the other corteges by the rules of genetic algorithms. Here the application of various genetic methods like the cross over is appropriate, when we group the former members of wrong corteges likely to the grouping of right corteges. For thus created the second version $\bar{S}_2$ of initial conditions we launch the repetition again and so on. It results in the sequence of pairs

$$(\bar{S}^1_{ini}, \bar{S}^1_{fin}), (\bar{S}^2_{ini}, \bar{S}^2_{fin}), \ldots \qquad (9.1)$$

where each pair $(\bar{S}^j_{ini}, \bar{S}^j_{fin})$ represent the digest of the repetition number j. The passage from one pair to the next consists of three steps: swarm evolution via impulse exchange, selection and the replication of right pairs. The exchange of impulses between the different corteges plays the role of mutations on the evolutionary programming. If we consider the swarm $\bar{S}$ as the world in the many world interpretation of quantum theory, the impulse exchange between the two corteges means the interaction between the different worlds. The chain 9.1 must be abrupt when the number of elements of the selected groups becomes stable.

We represent the argument for that the method of state selection lies along the core of standard quantum unitary dynamics for many particles. Let us turn to the Feynman path integrals (see [10]) where the wave function Ψ in each time instant t is determined by the following equation:

$$\Psi(t, \bar{r}) = \int\limits_{R^{3n}} K(t, \bar{r}, t_1, \bar{r}_1)\Psi(t_1, \bar{r}_1), \qquad (9.2)$$

where K is the kernel of our system, that can be treated as the amplitude careered by a cortege, if we assume that the samples carrier complex numbers amplitudes instead of their velocities as in the collective behavior method. Amplitudes K careered by

a cortege, thus depend on the initial and the final position $\bar{r}_1$ and $\bar{r}$, and must be then closed for the corteges which initial and final spatial positions are closed. Let us estimate the deposit to the probability $|\Psi(t, \bar{r})|^2$ of two groups of corteges with l elements each: the first group contains in the same group $\mathcal{G}_j$, and the corteges from the second group have only the final positions closed but the initial are different, and, for simplicity, randomly chosen. The deposits of these two groups to the probability are approximately

$$d_1 = |\sum_{s=1}^{l} \alpha|^2 = k^2|\alpha|^2, \quad d_2 = |\sum_{s=1}^{l} \alpha e^{i\phi_s} \approx k|\alpha|^2$$

where the phases ϕ_s are distributed randomly. The last approximate equality follows from the fact that for the uniform distribution of ϕ_s the medium of the distance of this sum from zero must have the order square root of the module of a summand. Hence, the deposit of the first group is prevailing. Returning to the samples in the collective behavior, we note that the complex amplitudes here are substantiated by the velocities of samples, and the deposit of minor groups $\mathcal{G}_j$ for $j > k_1$ will be much smaller than the deposit of the right samples taken in the same quantity, that legalizes the selection procedure, if we assume that the wave functions are continuous.

We illustrate the action of the genetic algorithm of state selection on our example with the association of protons in the molecular ion of hydrogen. We suppose that the initial state of the first proton and the atom of hydrogen are close sufficiently to the forming of molecular ion of hydrogen. We treat the electron not as the separate particle here, but as the factor which creates the attracting potential between protons. If the first choice of pairs (1 proton sample, 2 proton sample) is done such that many pairs were formed with the distance between protons far from the distance r_0 of stable molecular ion of hydrogen, then the protons from these pairs will fly to far distance one from another, and hence this pairs occur in the different groups. It results after several iterations in the growth of the groups where the initial distance between protons is close to r_0, and we obtain in the final the prevailing quantity of pairs which form the molecular ion of hydrogen.

In case when the initial positions of the first proton and the hydrogen atom are far, this scheme has to be extended. Here we must take into consideration also photons, which are emitted by this system and thus decrease its energy. Photons can be included to the scheme with quantum state selection as well. But the direct consideration of photons is not necessary, because we can replace them by some kind of friction, and split the time frame Δt to the smaller segments so that in the last segment the positions of flying proton and the target atom will be close enough to apply the selection procedure.

The simulation we have proposed touches the basic things in quantum mechanics. At first it factually utilises the fundamental idea of many worlds (Everett). Each cortege consisting of samples of the real particles represent the separate quantum world. The different worlds interact with each other, and the selection process plays the role of judge in this interaction. The interaction inself results from the mechanism of dynamical diffusion when the close corteges exchange their impulses on the fixed

place j. This exchange represents the exact form of the so called pre quantum fields considered in [6].

10. Conclusion

We propose the simple genetic algorithm for the simulation of association of atoms into molecules, based on the method of collective behavior. This algorithm is scalable in the sense that we can add new particles to the considered system and the construction still remains valid. In particular, it admits the inclusion of photons, and the complex molecules. The interesting peculiarity is that this algorithm can be reversed, the formal inversion, when we treat the dissociation process, gives us the picture of splitting of the molecule to the more simple molecules of atoms and we can estimate the probabilities of the both processes even for large quantity of participating atoms.

The description of association and dissociation of molecule based on the method of collective behavior is completely quantum and is based on Hilbert formalism. This tool is scalable and can be applied to the complex chemical processes. In particular we can expect that this approach is applicable to the explanation of the phenomenon of molecular memory detected in experiments.

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Statistical Reconstruction of Quantum States

We discuss a procedure of statistical reconstruction of quantum states. Multiparametric statistical model providing stable reconstruction of parameters by observations is considered. The only general method of this kind is the root model based on the representation of the probability density as a squared absolute value of a certain function, which is referred to as a psi-function in analogy with quantum mechanics. The psi-function is represented by an expansion in terms of an orthonormal set of functions. It is shown that the introduction of the psi-function allows one to represent the Fisher information matrix as well as statistical properties of the estimator of the state vector (state estimator) in simple analytical forms. The chi-square test is considered to test the hypotheses that the estimated vector converges to the state vector of a general population. The method proposed may be applied to its full extent to solve the statistical inverse problem of quantum mechanics (root estimator of quantum states). In order to provide statistical completeness of the analysis, it is necessary to perform measurements in mutually complementing experiments (according to the Bohr terminology).

The method of statistical estimation of the quantum state based on solving the likelihood equation and analyzing the statistical properties of the obtained estimates is developed. The developed approach applied to quantum-state reconstruction is based on the amplitudes of mutually complementary processes. The classical algorithm of statistical estimation based on the Fisher information matrix is generalized to the case of quantum systems obeying Bohr's complementarity principle. The maximum likelihood technique and likelihood equation are generalized in order to analyze quantum mechanical experiments. It is shown that the requirement for the expansion to be of a root kind can be considered as a quantization condition making it possible to choose systems described by quantum mechanics from all statistical models consistent, on average, with the laws of classical mechanics.

Introduction

The ability of measuring quantum states, no doubt, is of fundamental interest, because it provides a powerful tool for the analysis of basic concepts of quantum theory, such as the fundamentally statistical character of its predictions, the superposition principle, the Bohr's complementarity principle, etc. By the measurement of quantum state we will imply a data acquisition procedure followed by a computation procedure. The first step is a genuine measurement consisting of a set of operations under the representatives of a quantum statistical (pure or mixed) ensemble, as a result of which the experimenter acquires a set of

rates with which particular events occur. The second step consists of the mathematical procedure of reconstructing the quantum state of an object using the combination of the obtained statistical data.

The necessity of properly measuring the quantum states is dictated by the applied problems. For example, increase in the key distribution secrecy in quantum cryptography is associated with the increase in the dimensionality of Hilbert space for the states in use [1]; in this respect, certain hopes are pinned on the multi-level systems (qudits) [2, 3].

The development of technology of such multidimensional quantum systems as qudits (quantum dits), which are an alternative to more traditional two-level systems, qubits, promise significant advantages in problems of quantum informatics and cryptography. In particular, the use of qudits allows one to demonstrate a stronger violation of the Bell inequalities compared to systems based on qubits, which is of fundamental importance for quantum physics and quantum theory of information [4,5,6,7]. Much applied interest in qudit systems also comes from their possible use in quantum cryptography in key distribution problems [8,9].

Multilevel quantum systems prove to be more robust against unavoidable noise in communication channels. At the same time, the technology of preparation and measurement of qudits seems to be much more technically complicated than in the case of qubits. Efficient application of multilevel quantum systems in quantum cryptographic protocols requires secure complete high-precision control over quantum states. The possibility of such a high-precision control over three- and four-level single-mode polarized quantum states of biphotons was experimentally demonstrated for the first time in [10,11,12,13,14].

All these implementations belong to the art of the modern experimental technique and demonstrate the development of those quantum information branches relating to the practice. However, note that successful manipulation with quantum states implies the ability to control three important stages: state preparation, its transformation, and measurement. Quantum computation and communication systems should ensure the technology of preparation, transformation, and measurement of signals of a specific quantum-mechanical nature. The quantum signal determined by the vector of state in an abstract Hilbert space differs in principle from signals of the classical nature. An important distinctive feature of quantum signals compared to classical ones is the fundamental necessity of statistical description of their behavior. Technologically, the quantum state is determined by the procedure of its preparation. Such a procedure is termed the protocol. The protocol for the preparation of the quantum state specifies the quantum statistical ensemble that corresponds to it. This ensemble determines the potential possibility of generating an arbitrarily large number of representatives that are close to each other (ideally, identical). The measurement of an individual quantum object leads to a change in its quantum state (the wave function reduction); however, the experimenter deals not with a single object but with a large set of representatives of the quantum statistical ensemble. This particular feature leads to the situation that the traditional measurement procedures are necessarily replaced by measuring–computational algorithms, with the help of which experimentally obtained statistical data are subjected to a special mathematical processing aiming at reconstructing the parameters of the quantum state under study [15].

The methods of quantum tomography relate closely to the procedure of the classical tomography [16]. In [17] the technique of quantum tomography for the Wigner function based on the Radon transformation was suggested. A quantum-state reconstruction using the least-squares method was performed in [18]. The strategy of the maximal-likelihood method was suggested in Refs. [19,20]. Note that the maximal-likelihood method in the form which

automatically recovers the density matrices for a physical state (a density matrix must be Hermitian, positive, and semidefinite and have the unity trace) was developed in [21,22].

The advantages of the root estimation method are based on the ability to reconstruct the states in the Hilbert space of high dimensionality. The method is asymptotically effective, so it allows one to reconstruct the states with an accuracy that is most close to the accuracy achievable in principle. That is why the formalism applied to the unknown quantum states allowed us to formulate and experimentally check the fundamental statistical limits of the accuracy of state reconstruction [15,23,24].

The complete high-precision control over a quantum state requires taking into account statistical fluctuations and instrumental errors that arise in the course of realization of measuring–computational algorithms. The statistical fluctuations are connected with the fundamental quantum nature of the states under investigation and arise because the number of representatives of the quantum ensemble subjected to measurement is finite. As the observation time increases, the measurement process destroys the quantum states of an increasingly greater number of the ensemble representatives. Correspondingly, more and more exact information on the quantum state is extracted (the level of statistical fluctuations in the estimation of the vector of the quantum state becomes increasingly smaller) [25,26]. However, the accuracy level of the control over a quantum state cannot be arbitrarily high because of the occurrence of unavoidable technological restrictions and instrumental errors related to them (such as errors of the angle setting and errors of the parameters of polarization instruments, noise in the photon detection system, unstable operation of the pump laser, etc.) [27]. The theoretical consideration performed and the results of the mathematical modeling make it possible to determine technological requirements to the parameters of an experimental setup that are necessary for the secure high-precision control over the quantum state. The results of this study are important for the efficient practical realization of the elements and protocols of qudit- based quantum informatics.

1. Fisher information matrix and state estimator

A psi-function considered further is a mathematical object of statistical data analysis. The introduction of the psi-function implies that the "square root" of the probability density is considered instead of the probability density itself.

$$p(x) = |\psi(x)|^2$$

Let the psi function depend on S unknown parameters $c_0, c_1, ..., c_{s-1}$ (according to quantum mechanics, the basis functions are traditionally numbered from zero corresponding to the ground state). The parameters introduced are the coefficients of an expansion in terms of a set of basis functions. Assume that the set of the functions is orthonormal.

For the sake of simplicity, consider first a real valued psi function. Let an expansion have the form

$$\psi(x) = \sqrt{1 - \left(c_1^2 + ... + c_{s-1}^2\right)} \varphi_0(x) + c_1 \varphi_1(x) + ... + c_{s-1} \varphi_{s-1}(x). \tag{1}$$

Here, we have eliminated the coefficient $c_0 = \sqrt{1 - \left(c_1^2 + ... + c_{s-1}^2\right)}$ from the set of parameters to be estimated, since it is expressed via the other coefficients by the normalization condition.

The parameters $c_1, c_2, ..., c_{s-1}$ are independent. We will study their asymptotic behavior using the Fisher information matrix [28-29]

$$I_{ij}(c) = n \cdot \int \frac{\partial \ln p(x,c)}{\partial c_i} \frac{\partial \ln p(x,c)}{\partial c_j} p(x,c) dx$$

The fundamental significance of the Fisher information matrix consists in its property to set the constraint on achievable (in principle) accuracy of statistical estimators. According to the Cramer - Rao inequality [28-29], the matrix $\Sigma(\hat{\theta}) - I^{-1}(\theta)$ is nonnegative for any unbiased estimator $\hat{\theta}$ of an unknown vector valued parameter θ. Here, $\Sigma(\hat{\theta})$ is the covariance matrix for the estimator $\hat{\theta}$. The corresponding difference asymptotically tends to a zero matrix for the maximum likelihood estimators (asymptotic efficiency).

It is of particular importance for our study that the Fisher information matrix drastically simplifies if the psi function is introduced [23,24,30]

$$I_{ij} = 4n \cdot \int \frac{\partial \psi(x,c)}{\partial c_i} \frac{\partial \psi(x,c)}{\partial c_j} dx . \tag{2}$$

In the case of the expansion (1), the information matrix I_{ij} is $(s-1) \times (s-1)$ matrix of the form

$$I_{ij} = 4n \left(\delta_{ij} + \frac{c_i c_j}{c_0^2} \right), \qquad c_0 = \sqrt{1 - \left(c_1^2 + ... + c_{s-1}^2 \right)}. \tag{3}$$

A noticeable feature of the expression (3) is its independence on the choice of basis functions. Note that only the representation of the density in the form $p = |\psi|^2$ results in a universal (and simplest) structure of the Fisher information matrix.

In view of the asymptotic efficiency of the maximum likelihood estimators, the covariance matrix of the state estimator is the inverse Fisher information matrix:

$$\Sigma(\hat{c}) = I^{-1}(c) \tag{4}$$

Let us extend the covariance matrix by appending the covariance between the c_0 component of the state vector and the other components. In result, we find that the covariance matrix components are

$$\Sigma_{ij} = \frac{1}{4n} \left(\delta_{ij} - c_i c_j \right) \qquad i, j = 0,1,...,s-1 . \tag{5}$$

From the geometrical standpoint, the covariance matrix (5) is a second-order tensor. Moreover, the covariance matrix (up to a constant factor) is a single second-order tensor satisfying the normalization condition.

In quantum mechanics, the matrix

$$\rho_{ij} = c_i c_j \tag{6}$$

is referred to as a density matrix (of a pure state). Thus,

$$\Sigma = \frac{1}{4n} (E - \rho), \tag{7}$$

where E is the $s \times s$ unit matrix.

In the diagonal representation,

$$\Sigma = UDU^+ , \tag{8}$$

where U and D are unitary (orthogonal) and diagonal matrices, respectively.

As is well known from quantum mechanics, the density matrix of a pure state has the only (equal to unity) element in the diagonal representation. Thus, in our case, the diagonal of the D matrix has the only element equal to zero (the corresponding eigenvector is the state vector); whereas the other diagonal elements are equal to $\frac{1}{4n}$ (corresponding eigenvectors and their linear combinations form a subspace that is orthogonal complement to the state vector). The zero element at a principle diagonal indicates that the inverse matrix (namely, the Fisher information matrix of the S-th order) does not exist. It is clear since there are only $s-1$ independent parameters in the distribution.

The results on statistical properties of the state vector reconstructed by the maximum likelihood method can be summarized as follows. In contrast to a true state vector, the estimated one involves noise in the form of a random deviation vector located in the space orthogonal to the true state vector. The components of the deviation vector (totally, $s-1$ components) are asymptotically normal independent random variables with the same variance $\frac{1}{4n}$. In the aforementioned $s-1$-dimensional space, the deviation vector has an isotropic distribution, and its squared length is the random variable $\frac{\chi^2_{s-1}}{4n}$, where χ^2_{s-1} is the random variable with the chi-square distribution of $s-1$ degrees of freedom, i.e.

$$1 - \left(c, c^{(0)}\right)^2 = \frac{\chi^2_{s-1}}{4n}. \tag{9}$$

This expression means that the squared scalar product of the true and estimated state vectors is smaller than unity by asymptotically small random variable $\frac{\chi^2_{s-1}}{4n}$.

The results found allow one to introduce a new stochastic characteristic, namely, a confidence cone (instead of a standard confidence interval). Let ϑ be the angle between an unknown true state vector $c^{(0)}$ and that c found by solving the likelihood equation. Then,

$$\sin^2 \vartheta = 1 - \cos^2 \vartheta = 1 - \left(c, c^{(0)}\right)^2 = \frac{\chi^2_{s-1}}{4n} \leq \frac{\chi^2_{s-1,\alpha}}{4n}. \tag{10}$$

Here, $\chi^2_{s-1,\alpha}$ is the quantile corresponding to the significance level α for the chi-square distribution of $s-1$ degrees of freedom.

The set of directions determined by the inequality (10) constitutes the confidence cone. The axis of a confidence cone is the reconstructed state vector c. The confidence cone covers the direction of an unknown state vector at a given confidence level $P = 1 - \alpha$.

Root estimator provides refined representations of such classical results as chi-squared criterion and Gaussian approximation of binomial distribution.

Let $p_1, p_2, ..., p_s$ be theoretical probabilities, and $n_1, n_2, ..., n_s$ observed number of points fitting in corresponding intervals.

Thus, root form of chi-squared criterion is [24]:

$$4\left[n - \left(\sqrt{n_1 p_1} + \sqrt{n_2 p_2} + ... + \sqrt{n_s p_s}\right)^2\right] = \chi^2_{s-1}. \tag{11}$$

Eq.11 means that if probability distribution corresponds with the theoretical one, then the left value is random of chi-squared form with $s-1$ degrees of freedom. Chi-squared standard form [28] follows from chi-squared criterion of the form (11) (as an asymptotic limit).

$s = 2$ case corresponds to binomial distribution, and root-form approximation by normal distribution is:

$$2\left(\sqrt{n_1 p_2} - \sqrt{n_2 p_1}\right) \sim N(0,1) \tag{12}$$

where $p_1 + p_2 = 1$ $n_1 + n_2 = n$, $N(0,1)$- is a random value of standard normal form.

Similar result of classical theory of probability is the Moivre- Laplace theorem (see [28]):

$$\frac{n_1 - n p_1}{\sqrt{n p_1 p_2}} \sim N(0,1) \tag{13}$$

It is easy to ensure that eq. 13 asymptotically follows from eq.12. Nevertheless, for finite sample size approximation form (12) provides better accuracy compared to classical result (13) [15].

2. Statistical analysis of mutually complementing experiments

We have defined the psi function as a complex-valued function with the squared absolute value equal to the probability density. From this point of view, any psi function can be determined up to arbitrary phase factor $\exp(iS(x))$. In particular, the psi function can be chosen real-valued.

At the same time, from the physical standpoint, the phase of psi function is not redundant. The psi function becomes essentially complex valued function in analysis of mutually complementing (according to Bohr) experiments with micro objects [23,25].

According to quantum mechanics, experimental study of statistical ensemble in coordinate space is incomplete and has to be completed by study of the same ensemble in another (canonically conjugate, namely, momentum) space. Note that measurements of ensemble parameters in canonically conjugate spaces (e.g., coordinate and momentum spaces) cannot be realized in the same experimental setup.

The uncertainty relation implies that the two-dimensional density in phase space $P(x, p)$ is physically senseless, since the coordinates and momentum of micro objects cannot be measured simultaneously. The coordinate $P(x)$ and momentum $\widetilde{P}(p)$ distributions should be studied separately in mutually complementing experiments and then combined by introducing the psi function.

The coordinate-space and momentum-space psi functions are related to each other by the Fourier transform

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int \widetilde{\psi}(p) \exp(ipx) dp, \quad \widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int \psi(x) \exp(-ipx) dx. \tag{14}$$

Consider a problem of estimating an unknown psi function ($\psi(x)$ or $\widetilde{\psi}(p)$) by experimental data observed both in coordinate and momentum spaces. We will refer to this problem as an statistical inverse problem of quantum mechanics [23,25,26] (do not confuse it with an inverse problem in the scattering theory). The predictions of quantum mechanics are considered as a direct problem. Thus, we consider quantum mechanics as a stochastic theory, i.e., a theory describing statistical (frequency) properties of experiments with random events. However, quantum mechanics is a special stochastic theory, since one has to perform mutually complementing experiments (space-time description has to be completed by momentum-energy one) to get statistically full description of a population (ensemble). In

order for various representations to be mutually consistent, the theory should be expressed in terms of probability amplitude rather than probabilities themselves.

Methodologically, the method considered here essentially differs from other well known methods for estimating quantum states that arise from applying the methods of classical tomography and classical statistics to quantum problems [31,32,33]. The quantum analogue of the distribution density is the density matrix and the corresponding Wigner distribution function. Therefore, the methods developed so far have been aimed at reconstructing the aforementioned objects in analogy with the methods of classical tomography (this resulted in the term "quantum tomography") [16].

In [17], a quantum tomography technique on the basis of the Radon transformation of the Wigner function was proposed. The estimation of quantum states by the method of least squares was considered in [18]. The maximum likelihood technique was first presented in [19,20]. The version of the maximum likelihood method providing fulfillment of basic conditions imposed of the density matrix (hermicity, nonnegative definiteness, and trace of matrix equal to unity) was given in [21,22]. Characteristic features of all these methods are rapidly increasing calculation complexity with increasing number of parameters to be estimated and ill-posedness of the corresponding algorithms, not allowing one to find correct stable solutions.

The orientation toward reconstructing the density matrix overshadows the problem of estimating more fundamental object of quantum theory, i.e., the state vector (psi function). Formally, the states described by the psi function are particular cases of those described by the density matrix. On the other hand, this is the very special case that corresponds to fundamental laws in Nature and is related to the situation when the state described by a large number of unknown parameters may be stable and estimated up to the maximum possible accuracy.

Let us consider generalization of the maximum likelihood principle and likelihood equation for estimation of the state vector of a statistical ensemble on the basis of experimental data obtained in mutually complementing experiments. To be specific, we will assume that corresponding experiments relate to coordinate and momentum spaces.

We define the likelihood function as

$$L(x, p|c) = \prod_{i=1}^{n} P(x_i|c) \prod_{j=1}^{m} \widetilde{P}(p_j|c). \tag{15}$$

Here, $P(x_i|c)$ and $\widetilde{P}(p_j|c)$ are the densities in mutually complementing experiments corresponding to the same state vector c. We assume that n measurements were made in the coordinate space; and m, in the momentum one.

Then, the log likelihood function has the form

$$\ln L = \sum_{i=1}^{n} \ln P(x_i|c) + \sum_{j=1}^{m} \ln \widetilde{P}(p_j|c). \tag{16}$$

The maximum likelihood principle together with the normalization condition evidently results in the problem of maximization of the following functional:

$$S = \ln L - \lambda(c_i c_i^* - 1), \tag{17}$$

where λ is the Lagrange multiplier and

$$\ln L = \sum_{k=1}^{n} \ln(c_i c_j^* \varphi_i(x_k) \varphi_j^*(x_k)) + \sum_{l=1}^{m} \ln(c_i c_j^* \widetilde{\varphi}_i(p_l) \widetilde{\varphi}_j^*(p_l)). \tag{18}$$

Here, $\widetilde{\varphi}_i(p)$ is the Fourier transform of the function $\varphi_i(x)$.

Hereafter, we imply the summation over recurring indices numbering the terms of the expansion in terms of basis functions. On the contrary, statistical sums denoting the summation over the sample points will be written in an explicit form.

The necessary condition $\frac{\partial S}{\partial c_i^*} = 0$ for an extremum yields the likelihood equation

$$R_{ij} c_j = \lambda c_i \quad i, j = 0, 1, ..., s - 1 ,$$ (19)

where the R matrix is determined by

$$R_{ij} = \sum_{k=1}^{n} \frac{\varphi_i^*(x_k) \varphi_j(x_k)}{P(x_k)} + \sum_{l=1}^{m} \frac{\widetilde{\varphi}_i^*(p_l) \widetilde{\varphi}_j(p_l)}{\widetilde{P}(p_l)} .$$ (20)

The problem (19) is formally linear. However, the matrix R_{ij} depends on an unknown densities $P(x)$ and $\widetilde{P}(p)$. Therefore, the problem under consideration is actually nonlinear, and should be solved by the iteration method [23,24]. An exception is the histogram density estimator when the problem can be solved straightforwardly.

Multiplying both parts of Eq. (19) by c_i^* and summing with respect to i, we find that the most likely state vector c always corresponds to its eigenvalue $\lambda = n + m$ of the R matrix (equal to sum of measurements).

An optimal number of harmonics in the expansion is appropriate to choose, on the basis of the compromise, between two opposite tendencies: the accuracy of the estimation of the function approximated by a finite series increases with increasing number of harmonics, however, the statistical noise level also increases.

The likelihood equation in the root state estimator method has a simple quasilinear structure and admits developing an effective fast-converging iteration procedure even in the case of multiparametric problems. The numerical implementation of the proposed algorithm is considered by the use of the set of Chebyshev-Hermite functions as a basis set of functions [15,23,24].

The implication of the root estimator method to statistical reconstruction of optical quantum states is considered in [10,11,12,13,14].

Examples of mutually complementing experiments that are of importance from the physical point of view are diffraction patterns (for electrons, photons, and any other particles) in the near-field zone (directly downstream of the diffraction aperture) and in the Fraunhofer zone (far from the diffraction aperture). The intensity distribution in the near-field zone corresponds to the coordinate probability distribution; and that in the Fraunhofer zone, the momentum distribution. The psi function estimated by these two distributions describes the wave field (amplitude and phase) directly at the diffraction aperture. The psi function dynamics described by the Schrödinger equation for particles and the Leontovich parabolic equation for light allows one to reconstruct the whole diffraction pattern (in particular, the Fresnel diffraction).

In the case of a particle subject to a given potential (e.g., an atomic electron) and moving in a finite region, the coordinate distribution is the distribution of the electron cloud, and the momentum distribution is detected in a thought experiment where the action of the potential abruptly stops and particles move freely to infinity.

In quantum computing, the measurement of the state of a quantum register corresponds to the measurement in coordinate space; and the measurement of the register state after performing the discrete Fourier transform, the measurement in momentum space. A quantum

register involving n qubits can be in 2^n states; and correspondingly, the same number of complex parameters is to be estimated. Thus, exponentially large number of measurements of identical registers is required to reconstruct the psi function if prior information about this function is lacking.
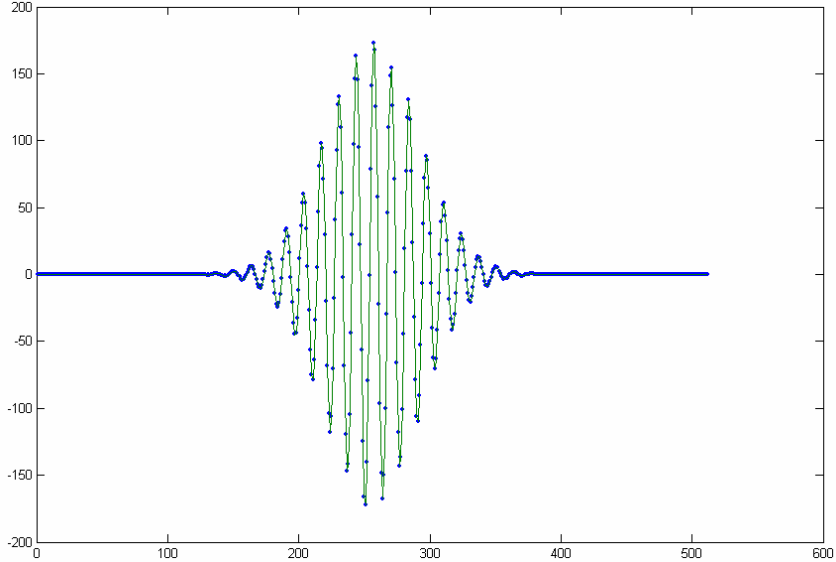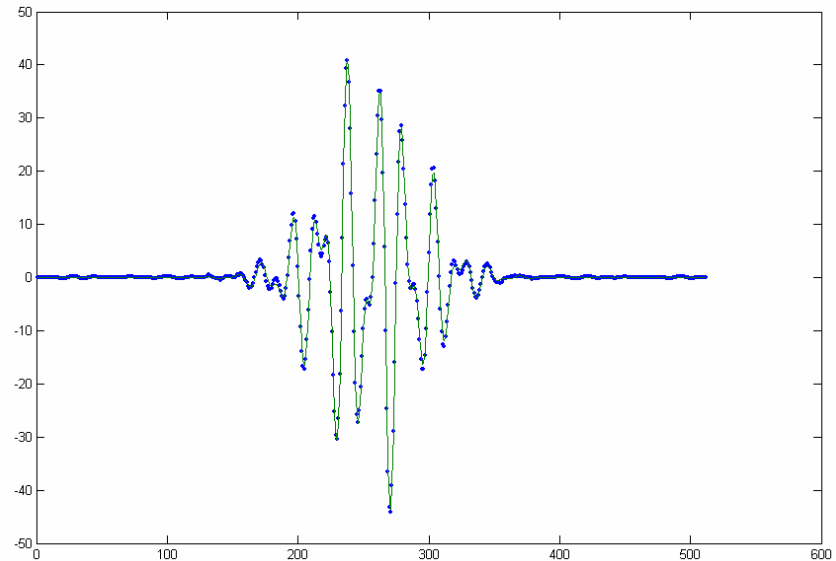
Fig. 1.a

Fig. 1.b

Fig. 1 Comparison between exact psi- function (solid line) and that estimated by a sample (dots); (a) real part, (b) imaginary part.

The state of quantum register is determined by the psi function

$$\psi = c_i |i\rangle \tag{21}$$

The probability amplitudes in the conjugate space corresponding to complementing measurements are

$$\widetilde{c}_i = U_{ij} c_j \tag{22}$$

The likelihood function relating to $n + m$ mutually complementing measurements is

$$L = \prod_i \left(c_i c_i^* \right)^{n_i} \prod_j \left(\widetilde{c}_j \widetilde{c}_j^* \right)^{m_j} \tag{23}$$

Here, n_i and m_j are the number of measurements made in corresponding states. In the case under consideration, the likelihood equation similar to (19) has the form

$$\frac{1}{n+m} \left[\frac{n_i}{c_i^*} + \sum_j \frac{m_j U_{ji}^*}{\widetilde{c}_j^*} \right] = c_i \tag{24}$$

An example of reconstruction of the state vector from the analysis of mutually complementary coordinate and momentum distributions is shown in Figure 1. We consider a quantum register: 9 qubits, $2^9 = 512$ states. In each experiment, the sample size is 10^6 representatives. This quantum state is reconstructed with the fidelity of $F = \left| \langle c_0 | c \rangle \right|^2 = 0.9999073$.

3. Process amplitudes and event generation intensity

The approach based on the use of psi-function is limited, in general by problems of non-relativity quantum mechanics. A more general approach is based on implementing a scattering matrix (S-operator)) [34]. Rigorously, problems of light interaction with matter, and photon field reconstruction, in particular, must be considered in this formalism framework [10,12]

Let S - operator that sets transformation of in-state to out-state.

$$\Phi_{out} = S\Phi_{in} \tag{25}$$

Let out-state be decomposed with a set of basis states

$$\Phi_{out} = c_j |j\rangle \tag{26}$$

Experimental study of quantum out-state transits to the study of mutually complementary quantum processes. The processes' amplitude is

$$M_{ij} = \langle j|S|i\rangle \tag{27}$$

Process amplitude square module specifies the intensity of event generation:

$$\lambda_j = M_j^* M_j \tag{28}$$

The event-generation intensity λ_j is the main quantity accessible for the measurement (λ_j is measured in frequency units (Hz).). The number of events occurring in any given time interval obeys the Poisson distribution. Therefore, the quantities λ_j specify the intensities of the corresponding mutually complementary Poisson processes and serve as estimates of the Poisson parameters (see below).

Although the amplitudes of the processes cannot be measured directly, they are of the greatest interest as quantities describing the fundamental relationships of quantum physics. From the superposition principle, it follows that the amplitudes are linearly related to the state-vector components. It is the purpose of quantum tomography to reproduce the amplitudes and state vectors which are hidden from the direct observation.

In some sense, the process amplitude is the "root " of the event generation intensity, likewise as ordinary psi-function is the "root" of probability density.

The linear transformation of the state vector c into the amplitude of the process M is described by a certain matrix X. Then the set of all amplitudes of the processes can be expressed by a single matrix equation

$$Xc = M \tag{29}$$

We call the matrix X the instrumental matrix of a set of mutually complementary measurements, by analogy with the conventional instrumental function. The matrix X is known *a priori* (before the experiment). Concrete examples of instrumental matrices applied to the problems of quantum optics can be found in [10,12,13,14,27]

In eq.29 state vector is proposed to be non-normalized. The usage of non-normalized vector releases us from inserting an interaction constant in (29). The vector c norm, obtained as the result of quantum system reconstruction, provides information of total intensity of all the processes considered in the experiment.

Now let us consider maximum likelihood estimator of state vector. The likelihood function is defined by the product of Poisson probabilities:

$$L = \prod_i \frac{(\lambda_i t_i)^{k_i}}{k_i!} e^{-\lambda_i t_i} \tag{30}$$

where k_i is the number of coincidences observed in the i th process during the exposure time t_i, and λ_i are the unknown theoretical event-generation intensities.

The log likelihood (logarithm of the likelihood function) is, except for an insignificant constant,

$$\ln L = \sum_i \left(k_i \ln(\lambda_i t_i) - \lambda_i t_i \right) \tag{31}$$

We also introduce the matrices with elements defined by the following formulas:

$$I_{js} = \sum_i t_i X_{ij}^* X_{is} \tag{32}$$

$$J_{js} = \sum_i \frac{k_i}{\lambda_i} X_{ij}^* X_{is} \quad i,s = 1,2,3 \tag{33}$$

The matrix I is determined from the experimental protocol. We shall call it hermitian matrix of Fisher information. On the contrary, the matrix J is determined by the

experimental values of k_i and by the unknown event-generation intensities λ_i Let us call it empirical matrix of Fisher information (see also Section 4).

In terms of these matrices, the condition for the extremum of function (20) can be written as

$$Ic = Jc \tag{34}$$

whence it follows that

$$I^{-1}Jc = c \tag{35}$$

We will call the latter relationship the likelihood equation. This is a nonlinear equation, because λ_i depends on the unknown state vector c. Because of the simple quasi-linear structure, this equation can easily be solved by the iteration method [23,24]. The operator $I^{-1}J$ can be called quasi- identity operator. Note that it acts as the identical operator on only one vector in the Hilbert space, namely, on the vector corresponding to solution (35) and representing the maximum possible likelihood estimate for the state vector. The condition for existence of the matrix I^{-1} is a condition imposed on the initial experimental protocol. The resulting set of equations automatically includes the normalization condition, which is written as

$$\sum_i k_i = \sum_i \left(\lambda_i t_i \right) \tag{36}$$

This condition implies that, for all processes, the total number of detected events is equal to the sum of the products of event detection rates into the exposure time.

4. Statistical fluctuations of state vector of quantum system

As already mentioned before, state vector with undefined primary norm provides the most complete information of the system. Fluctuations of quantum state (and norm fluctuations, in particular) in a normally functioning quantum information system should be within certain range, defined by statistical theory. This section is devoted to that problem.

Practical significance of accounting statistical fluctuations in quantum system deals with developing methods of estimation and control of precision and stability of quantum information system functioning, and also methods of detecting external interception to the system (Eve attack on the quantum channel between Alice and Bob).

The estimate of the non-normalized state vector c, obtained by the maximum likelihood principle, differs from the exact state vector $c^{(0)}$ by a random value $\delta c = c^{(0)} - c$. Let us consider statistical properties of the fluctuation vector δc by expansion of the log likelihood function near the stationary point. The expansion is as follows:

$$-\delta \ln L = \left[\frac{1}{2} \left(K_{sj} \delta c_s \delta c_j + K_{sj}^* \delta c_s^* \delta c_j^* \right) + I_{sj} \delta c_s^* \delta c_j \right], \tag{37}$$

where together with the above (in (32)) defined hermitian matrix of Fisher information I, we define a symmetric Fisher information matrix K, which elements are defined by the following equation:

$$K_{sj} = \sum_\nu \frac{\lambda_\nu t_\nu}{M_\nu^2} X_{\nu s} X_{\nu j} \tag{38}$$

where M_ν is the amplitude of the ν - th process.

K in general case is a complex symmetric (non-hermitian) matrix.

From all the possible fluctuations let us mark out the so-called gauge fluctuations. Infinitesimal global gauge transformations of a state vector are as follows:

$$\delta c_j = i\varepsilon\, c_j, \quad j = 1,2,...,s \tag{39}$$

where ε - is an arbitrary small real number, s - the Hilbert space dimension.

Evidently, for gauge transformations $\delta \ln L = 0$. It means that two states vectors that differ by a gauge transformation, are statistically equivalent (have the same likelihood). Such vectors are equivalent physically too (global state vector phase is physically non-observable). From statistical point of view, the set of mutually complementing measurements should be chosen in a manner that for all the other fluctuations (except gauge) the equation (37) is strictly positive: $-\delta \ln L > 0$. We shall call this inequality the statistical completeness condition of a set mutually complementing measurement. Let us obtain constructive criteria of statistical completeness of measurements. The complex fluctuation vector δc is convenient to be represented by a real vector of double length. Let us extract explicitly the real and the imaginary parts of the fluctuation vector $\delta c_j = \delta c_j^{(1)} + i\delta c_j^{(2)}$ and transit from the complex vector δc to the real $\delta\xi$

$$\delta c = \begin{pmatrix} \delta c_1 \\ \delta c_2 \\ \vdots \\ \delta c_s \end{pmatrix} \to \delta\xi = \begin{pmatrix} \delta c_1^{(1)} \\ \vdots \\ \delta c_s^{(1)} \\ \delta c_1^{(2)} \\ \vdots \\ \delta c_s^{(2)} \end{pmatrix} \tag{40}$$

In particular for qutrits ($s = 3$) this provides transition from 3-component complex vector to 6-component real vector.

In the new representation the equation (37) is expressed in the form:

$$\delta \ln L = -H_{sj}\delta\xi_s\delta\xi_j = -\langle \delta\xi | H | \delta\xi \rangle, \tag{41}$$

where the matrix H we shall call the complete information matrix. It is of the following block form:

$$H = \begin{pmatrix} \mathrm{Re}(I+K) & -\mathrm{Im}(I+K) \\ \mathrm{Im}(I-K) & \mathrm{Re}(I-K) \end{pmatrix} \tag{42}$$

Matrix H is real and symmetric. It is of double dimension to matrices I and K.

Now for one it is easy to formulate the desired characteristic condition of mutually complementing measurement set completeness. For a set of measurements to be statistically complete, it is necessary and sufficient that one (and the only one) eigenvalue of the complete information matrix H is equal to zero, while the other are strictly positive.

Notice that by checking the condition, one not only verifies statistical completeness of a measurement protocol but also, insures that the obtained extremum is of maximum likelihood.

Eigenvector that has eigenvalue equal to zero corresponds to gauge fluctuation direction (such fluctuations are of no physical importance as stated above). Eigenvectors corresponding to the other eigenvalues specify in Hilbert space directions that we shall call principle state vector fluctuation directions.

Principle fluctuations variance is

$$\sigma_j^2 = \frac{1}{2h_j}, \qquad j = 1,...,2s-1 \qquad (43)$$

where h_j is the eigenvalue of the information matrix H, corresponding to the j-the principle direction.

The most critical direction in Hilbert space is the one with the maximum variance σ_j^2, while the eigenvalue h_j is accordingly minimal. The knowledge of numeric dependences of statistical fluctuations allows researcher to estimate distributions of various statistical characteristics.

The most important information criterion that specifies the general possible level of statistical fluctuations in quantum information system is the chi-square criterion. According to the stated above it can be expressed as:

$$2\langle \delta\xi | H | \delta\xi \rangle \sim \chi^2(2s-1) \qquad (44)$$

where s is the Hilbert space dimension

Equation (44) has the meaning that the left value, that describes the level of state vector information fluctuations is of chi-square distribution with $2s-1$ degrees of freedom.

The validity of the analytical expression (44) is justified by the results of numerical modeling and observed data (see [11,12]). Similarly to (40) let us introduce the transformation of a complex state vector to a real vector of double length:

$$c = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_s \end{pmatrix} \rightarrow \xi = \begin{pmatrix} c_1^{(1)} \\ \vdots \\ c_s^{(1)} \\ c_1^{(2)} \\ \vdots \\ c_s^{(2)} \end{pmatrix} \qquad (45)$$

It can be shown that the information carried by a state vector is equal to double total number of observations in all processes.

$$\langle \xi | H | \xi \rangle = 2n, \qquad (46)$$

where $n = \sum_v k_v$

Then, the chi-square criterion can be expressed in the form invariant to the state vector scale (let us remind that we consider a non-normalized state vector).

$$\frac{\langle \delta\xi | H | \delta\xi \rangle}{\langle \xi | H | \xi \rangle} \sim \frac{\chi^2(2s-1)}{4n} \qquad (47)$$

Equation (47) describes distribution of relative informational fluctuation. It shows that relative information uncertainty of a quantum state decreases with number of observations as $1/n$.

The mean value of relative information fluctuation is:

$$\frac{\overline{\langle \delta\xi | H | \delta\xi \rangle}}{\langle \xi | H | \xi \rangle} = \frac{2s-1}{4n} \qquad (48)$$

As a measure of correspondence of a theoretical state vector and its' estimate let us introduce a characteristic, that we shall call informational fidelity.

$$F_H = 1 - \frac{\langle \delta\xi | H | \delta\xi \rangle}{\langle \xi | H | \xi \rangle} \tag{49}$$

Value $1 - F_H$ we shall call informational loss.

The convenience of informational fidelity F_H is enclosed in its' simpler statistical properties compared to the conventional one F. For a system where statistical fluctuations are dominant fidelity is a random value, based on chi-square distribution .

$$F_H = 1 - \frac{\chi^2(2s-1)}{4n}, \tag{50}$$

where $\chi^2(2s-1)$ is a random value of chi-square type with $2s-1$ degrees of freedom.

Informational fidelity value asymptotically tends to unity with sample size growth, while informational loss tends to zero. Complementary (to statistical fluctuations) noise decreases informational fidelity level compared to the theoretical level (50).

The examples of applying the theory to quantum optical state reconstruction can be found in [10,11,12,13,14].

In [27] is considered a model that approximately takes into account instrumental errors in problems of precision reconstruction of quantum states. The model is based on the notion of coherence volume, which characterizes the quality of the experimental and technological realization of the measurement protocol of a quantum state. Various sources of instrumental errors that affect the reconstruction accuracy of quantum states are mathematically modeled. The objective of [27] is to systematically study the effect of various instrumental errors on the quantum state reconstruction accuracy. The study is performed by using as an example the protocol for the measurement of four-level polarization quantum states of biphotons that we experimentally realized in [14].

5. Root estimator and quantum dynamics

Assume that the mechanical equations are satisfied only for statistically averaged quantities (the averaged Newton's second law of motion)

$$\frac{d^2}{dt^2}\left(\int P(x)\vec{x}\,dx\right) = -\frac{1}{m}\left(\int P(x)\frac{\partial U}{\partial \vec{x}}\,dx\right) \tag{51}$$

Let us require the density $P(x)$ to admit the root expansion [23,24] (s components), i.e.,

$$P(x) = \left|\psi^{(1)}(x)\right|^2 + \left|\psi^{(2)}(x)\right|^2 + ... + \left|\psi^{(s)}(x)\right|^2, \tag{52}$$

where

$$\psi^{(l)}(x) = c_j^{(l)}(t)\varphi_j(x) \qquad l = 1,..,s \tag{53}$$

We will search for the time dependence of the expansion coefficients in the form of harmonic dependence

$$c_j^{(l)}(t) = c_{j0}^{(l)}\exp(-i\omega_j t). \tag{54}$$

Then, Eq. (51) yields

$$m(\omega_j - \omega_k)^2 \sum_{l=1}^{s} c_{j0}^{(l)} c_{k0}^{*(l)} \langle k | \vec{x} | j \rangle \exp(-i(\omega_j - \omega_k)t) =$$
$$= \sum_{l=1}^{s} c_{j0}^{(l)} c_{k0}^{*(l)} \langle k | \frac{\partial U}{\partial \vec{x}} | j \rangle \exp(-i(\omega_j - \omega_k)t) \qquad (55)$$

Here, the summation over recurring indices j and k is meant. The matrix elements in (55) are determined by the formulas

$$\langle k | \vec{x} | j \rangle = \int \varphi_k^*(x) \vec{x} \, \varphi_j(x) dx \qquad (56)$$

$$\langle k | \frac{\partial U}{\partial \vec{x}} | j \rangle = \int \varphi_k^*(x) \frac{\partial U}{\partial \vec{x}} \varphi_j(x) dx \qquad (57)$$

In order for the expression (55) to be satisfied at any instant of time for arbitrary initial amplitudes, the left and right sides are necessary to be equal for each matrix element. Therefore,

$$m(\omega_j - \omega_k)^2 \langle k | \vec{x} | j \rangle = \langle k | \frac{\partial U}{\partial \vec{x}} | j \rangle \qquad (58)$$

This expression is a matrix equation of the Heisenberg quantum dynamics in the energy representation (written in the form similar to that of the Newton's second law of motion). The basis functions and frequencies satisfying (58) are the stationary states and frequencies of a quantum system, respectively (in accordance with the equivalence of the Heisenberg and Schrödinger pictures).

Indeed, let us construct the diagonal matrix from the system frequencies ω_j. The matrix under consideration is Hermitian, since the frequencies are real numbers. This matrix is the representation of a Hermitian operator with eigenvalues ω_j, i.e.,

$$H | j \rangle = \hbar \omega_j | j \rangle \qquad (59)$$

Let us find an explicit form of this operator. In view of (59), the matrix relationship (58) can be represented in the form of the operator equation

$$\left[H[Hx] \right] = \frac{\hbar^2}{m} \hat{\partial} U, \qquad (60)$$

where $\hat{\partial} = \frac{\partial}{\partial x}$ is the operator of differentiation and $[\ ]$, the commutator.

The Hamiltonian of a system

$$H = -\frac{\hbar^2}{2m} \hat{\partial}^2 + U(x) \qquad (61)$$

is the solution of operator equation (60).

Let us consider density matrix with the elements:

$$\rho_{jk} = \sum_{l=1}^{s} c_j^{(l)} c_k^{*(l)} = \sum_{l=1}^{s} c_{j0}^{(l)} c_{k0}^{*(l)} \exp(-i(\omega_j - \omega_k)t) \qquad (62)$$

Basing on the above results one can easily derive the equation for density matrix dynamics, usually called quantum Liouville equation.

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho] \tag{63}$$

Thus, if the root density estimator is required to satisfy the averaged classical equations of motion, the basis functions and frequencies of the root expansion cannot be arbitrary, but have to be eigenfunctions and eigenvalues of the system Hamiltonian, respectively.

The relationships providing that the averaged equations of classical mechanics are satisfied for quantum systems are referred to as the Ehrenfest equations [35]. These equations are insufficient to describe quantum dynamics. As it has been shown above, an additional condition allowing one to transform a classical system into the quantum one (i.e., quantization condition) is actually the requirement for the density to be of the root form.

Thus, if we wish to turn from the rigidly deterministic (Newtonian) description of a dynamical system to the statistical one, it is natural to use the root expansion of the density distribution to be found, since only in this case a stable statistical model can be found. On the other hand, the choice of the root expansion basis determined by the eigenfunctions of the energy operator (Hamiltonian) is not simply natural, but the only possible way consistent with the dynamical laws.

Conclusions

Let us state a short summary.

Search for multiparametric statistical model providing stable estimation of parameters on the basis of observed data results in constructing the root density estimator. The root density estimator is based on the representation of the probability density as a squared absolute value of a certain function, which is referred to as a psi-function in analogy with quantum mechanics. The method proposed is an efficient tool to solve the basic problem of statistical data analysis, i.e., estimation of distribution density on the basis of experimental data.

The coefficients of the psi-function expansion in terms of orthonormal set of functions are estimated by the maximum likelihood method providing optimal asymptotic properties of the method (asymptotic unbiasedness, consistency, and asymptotic efficiency). The introduction of the psi-function allows one to represent the Fisher information matrix as well as statistical properties of the sate vector estimator in simple analytical forms. Basic objects of the theory (state vectors, information and covariance matrices etc.) become simple geometrical objects in the Hilbert space that are invariant with respect to unitary (orthogonal) transformations.

A new statistical characteristic, a confidence cone, is introduced instead of a standard confidence interval. The chi-square test is considered to test the hypotheses that the estimated vector equals to the state vector of general population.

The root state estimator may be applied to analyze the results of experiments with micro objects as a natural instrument to solve the inverse problem of quantum mechanics: estimation of state vector by the results of mutually complementing (according to Bohr) measurements (processes). Generalization of the maximum likelihood principle to the case of statistical analysis of mutually complementing experiments is proposed.

On the basis of fundamental statistical principles, the theory of statistical fluctuations of quantum system state vector is developed. The concept of Fisher informational matrix for a set of mutually- complementing quantum processes is introduced. The condition for statistical completeness is formulated. A comparison of the reconstruction results with the

fundamental statistical level of accuracy can serve as a basis for some problems such as the set-up adjustment, operation stability control, revelation of foreign interference in the quantum system, etc.

It is shown that the requirement for the density to be of the root form is the quantization condition. Actually, one may say about the root principle in statistical description of dynamic systems. According to this principle, one has to perform the root expansion of the distribution density in order to provide the stability of statistical description. On the other hand, the root expansion is consistent with the averaged laws of classical mechanics when the eigenfunctions of the energy operator (Hamiltonian) are used as basis functions. Figuratively speaking, there is no a regular statistical method besides the root one, and there is no regular statistical mechanics besides the quantum one.

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Numerical method of entangled state selection in association of molecules[*]

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We represent the economy method of separation of the entangled states of GHZ and W types which arise in the process of association of a single molecule. It makes possible to separate these types of quantum states in the simulation of real processes like the association of molecular ion of hydrogen by means of existing computers with the strictly limited memory. Numerical realization of this method is in process; we represent the semiclassical part of it, that is based on Landau-Ziner description of the association of molecules. Results of statistical processing of the row of numerical experiments are shown.

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1. Introduction and background

The rapid development of quantum computing in the past twenty years reveals two main tensions. The first: maintaining of the QC technology and theoretical support in the construction of quantum processors, and the second: elaboration of programming tools and media for the main aim of QC project: the simulation of real many particle quantum processes (see [1],[2],[8]). In the second direction we must find the best algorithmic surrounding of a quantum processor that makes possible to outperform the velocity of classical supercomputers in the simulation problems (see [3],[4]). For this aim we need to determin in details which computational tasks in quantum dynamics really require quantum computer, and which can be fulfilled effectively without it. For example, we can mention that entanglement cannot serve as the criterion of that QC exclusively is needed for the quantum state description ([9]). Many entangled states can be easily described by the c! lassical computational means, the most known example is GHZ and W states ([12]). To find such computational terms one needs to exploit the idea of grained space ([5],[6]), and use the more advanced algorithmic ideas. We note that algorithm approach cannot be reduced to the naive idea (see [7]) of the replacement of exact mathematical solutions to the fuzzy simple forms of mechanical representation. The idea of algorithmic approach is found on the valid fundament of the constructive mathematics.

Nevertheless, to realize it practically we need the reliable and, as possible, simple simulating programs that would use the ideas of classical simulation as well as

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quantum approach. The main obstacle in QC technology - decoherence - can be represented in the computer simulation as the severe limitation of the classical memory (see [3], [4]).

In this paper we represent one simple method of simulation of the scattering reactions which can help us to determin quantitatively the role of entanglement in chemistry.

2. GHZ and W states and its role in chemistry

We choose GHZ and W states as the most known example of states with the highest level of entanglement which at the same time plays the serious role in chemistry. GHZ states represent the quantum motion of a molecule as a whole, and W states represent the internal oscillations of the separate atoms in a molecule. It is worth noting that we focuse only on these embodiment of two abstract types of quantum states, whereas they have also the other realizations: entanglement of the excited states of ions in Paul trap, Cooper pairs of electrons in superconductors, etc. Chemical reactions give the reach area where the application of quantum entanglement is very important. The absence of a robust computer simulator of chemical reactions evidences about the crucial role of quantum entanglement in the dynamics of association of molecules.

These quantum states have the form

$$
\begin{aligned}
GHZ: \quad & \lambda_1|11\ldots1\rangle + \lambda_2|22\ldots2\rangle + \ldots + \lambda_k|kk\ldots k\rangle, \\
W: \quad & \lambda_1|100\ldots0\rangle + \lambda_2|010\ldots0\rangle + \ldots + \lambda_k|00\ldots1\rangle.
\end{aligned}
\tag{2.1}
$$

We introduce the measure of entanglement of the state Ψ of bipartite system $S = S_1 \cup S_2$, $S_1 \cap S_2 = \emptyset$ as von Neyman quantum entropy $E_{\Psi,S_1,S_2} = Tr(\rho_{S_2} \ln \rho_{S_2}) = Tr(\rho_{S_1} \ln \rho_{S_1})$ for partial density matrix ρ_{S_2}. For a system S with many parts we define the measure of entanglement as

$$
E_\Psi = min_{S_1,S_2: \ S=S_1\cup S_2, \ S_1\cap S_2=\emptyset} E_{\Psi,S_1,S_2}.
\tag{2.2}
$$

The different entangled measure are known, for example, Akulin measure of tanglemeter (see [9]), but for our aims here it is not significant.

These states is have the maximal measure of entanglement in some vicinity of them in Hilbert space. Hence, the practical fabrication of such states is important for quantum computers and inforation processing. These states are already fabricated in experiments with ions in Paul trap. We will show how these states can be selected by simple and economical algorithm in course of the simulation of process of molecule association.

3. Problem of quantum state selection

Here we define the process of the selection of quantum states in the numerical experiments. We start with the semiclassical description of the process of scattering of one abstract particle, called the bullet, on the other, called the target. We always write the parameters of them in this order.

One separate particle can be classically represented as the point with some atributes (mass, charge, spin, etc.). This representation is called a (classical) sample of the particle. A sample has its own trajectory as a classical particle. If we treat the particle as the quantum one, it means that we represent it as the ensemble of its classical samples. The density of samples is given by

$$\rho(\bar{x}) = \lim_{\delta x \longrightarrow \infty} \frac{N(\bar{x}, \delta x)}{\delta x^3}. \tag{3.1}$$

The main property of density which connect it with quantum mechanics is Born rule:

$$|\Psi(\bar{x})|^2 = \rho(\bar{x}). \tag{3.2}$$

In principal, the last equation can be chosen as the definition of ensemble representation of the wave function. This is sufficient for the representation of quantum dynamics via Feynman path integrals. We suppose that each sample moves along its own trajectory and scopes the amplitude λ depending on the action of this sample according the formula

$$\lambda(t_1) = e^{-\frac{iS(\gamma, t_0, t_1)}{h}}, \quad S(\gamma, t_0, t_1) = \int\limits_{t_0}^{t_1} (E_{kin} - E_{pot})dt, \tag{3.3}$$

where E_{kin}, E_{pot} is the kinetic and the potential energy of the sample. The resulting wave function is calculated by the summing of all amplitudes λ on all samples which occure in the small vicinity of the corresponding point in the corresponding time instant (see [10]).

Alternatively, we can use the mechanism of dynamical diffusion on the ensemble of samples. This mechanism includes the change of impulses between the near neigboring samples which otherwise preserve their speeds. The dynamical diffusion mechanism ensures the admissible approximation of quantum dynamics after the fixation of appropriate grain of spatial resolution (see [3]). At last we could choose the other algorithm for determiming of individual trajectories: from the method of quantum pseudo potential (see [11]), to the semiclassical representation of separate particles as the wave packages of Gauss form (see [12]). We agree that the choice of individual trajectories for the separate samples are somehow chosen.

We now consider the joint state of two real quantum particles: the bullet and the target in the framework of quantum Hilbert formalism for many particles. In Hilbert quantum formalizm it has the general form

$$\sum_{j,l} \lambda_{j,l} |\bar{x}_j, \bar{x}_l\rangle \tag{3.4}$$

where $|\bar{x}_j\rangle$ and $|\bar{x}_l\rangle$ are the coordinates of the target and bullet correspondingly. The pair $|\bar{x}_j, \bar{x}_l\rangle$ is the basic state of the joint system, formed by the bullet and the target. Unitary evolution of this system determined by Shroedinger equation contains

two operators acting sequentially at each time frame: the operator of kinetic energy $(-\frac{h^2}{2m}\Delta_{bul})\bigotimes(-\frac{h^2}{2m}\Delta_{tar})$, where Laplace operators Δ act independently to each of our two particles, and the operator of potential energy $V(\bar{x}_{bul}, \bar{x}_{tar})$ that acts on both particles simultaneously.

For the ensemble representation of quantum evolution it means that the action of operator of the kinetic energy must be ensured by internal process in the ensembles of samples corresponding to the bullet and to the target separately, whereas the action of the operator of the potential energy must be ensured by the interaction between the samples belonging to the different ensembles.

We assume that the model of evolution in the separate ensemble of the samples is such that we can trace the trajectory of each sample (Feynman path integrals do not completely satisfy this condition, but it can be modify by the artificial details to fit it). We then can choose randomly one sample from one ensemble, the second sample from the second ensemble, and follow their history that includes the independent influence from the other samples of these ensembles to each chosen sample, and interactions between these two samples only. In the other words, all interactions between two real quantum particles can be reduced to the interactions inside of one pair of its samples chosen randomly. If L is the total number of the samples in each ensemble, we have L^2 possible pairs of two samples. For n real quantum particles we will have corteges of the form $a_1, a_2, \ldots, a_n$ of their samples instead of the pairs. If the number of real particles grows the number of all corta! ges grows as L^n that is the reflection of the main computational problem of quantum theory of many bodies.

Therefore, for the computer simulation of quantum many body dynamics the following problem arises: how to select the "significant" corteges $a_1, a_2, \ldots, a_n$ of the samples which gather the bulk of amplitude. Let $\mathcal{B}$ be the set of all cortages $a_1, a_2, \ldots, a_n$. The selection problem is then to find the small (not exponentially large) subset $B \subset \mathcal{B}$ such that $\int_B |\Psi(\bar{x})|^2 \, d\bar{x} > 1 - \epsilon$ for the chosen error probability ϵ. We call the finding of such set B the problem of state selection. In case when the valuable part of B consists of entangled states of some type Z, the problem of state selection can be called the problem of selection of states of type Z. If for some class of quantum many body evolutions, foor its states Z the set B can be obtained by some effective algorithm, we say that for the class Z the problem of state selection is solved constructively. Here we assume that the initial set of states for the evolutions from Z are simply designed (can be obtained by the effective — polynomial time classical algorithms).

We note that the problem of state selection not mandatory has the solution for every reasonable quantum evolution in the whole Hilbert space. For example, it is certainly unsolvable for the fast quantum algorithms, which the key property is the distribution of the amplitude among the exponentially large number of states. Fast quantum algorithms is not the sole example: even for Walsh-Hadamard transform $H^{\otimes n}$ for Hadamard operator H this distribution of amplitude takes place. Nevertheless, we have reasons to expect that for some kinds of quantum evolution the selection problem can be solved constructively. One of such a class is the class of quantum mechanical systems which Lagranjian has the quadratic form $L = \bar{a}\bar{x}^2 + \bar{b}\bar{x}\bar{x}_t + \bar{c}\bar{x}_t^2$

of coordinates and impulses (for example, the system of quantum pendulums). It is proved in [10] that for such systems all trajectories with significant deposit to the amplitudes are classical ! trajectories, that immediately gives us the effective method of state selection, because we simply have to trace all trajectories generated by the easy algorithm.

Problem of state selection is important also for quantum computing. Its solution establishes the specific upper bound for the quantum evolutions which yet can be simulated classically, e.g. the simulation of evolutions lying beyond this border requires quantum computer. Up to nowadays, fast quantum algorithms represent engenious constructions, and by solving of the state selection problem we could try to find the more practical examples of fast quantum evolutions which themselves can serve as fast quantum subroutine in the simulation of complex systems. Such quantum subroutine can be found among the evolutions which do not admit the effective state selection.

4. Robust algorithm for quantum state selection

We now show how the problem of quantum state selection can be solved for the wide class of quantum evolutions. We will not define this class exactly, this is the subject of the further work. The robustness of our algorithm lies in its simple form and conveniency for programming.

We describe the algorithm on our simple example with the bullet and the target. We start from the subset $B_0 \subset \mathcal{B}$ that is obtained by the randomply chosen partner a — the sample of the target for each sample of the bullet b. This set B_0 represents nonentangled state which we initially have in the starting point. We have $B_0 = \{(a_1, b_1), (a_2, b_2), \ldots, (a_n, b_n)\}$.

Let us consider the evolution operator which acts on B_0 naturally:

$$B_0 \longrightarrow B_1 = \tilde{B}_0 = \{(\tilde{a}_1, \tilde{b}_1), (\tilde{a}_2, \tilde{b}_2), \ldots, (\tilde{a}_n, \tilde{b}_n)\}. \tag{4.1}$$

We now group all the pairs from B_1 in the several quantity of groups: $\Gamma_1, \Gamma_2, \ldots$, such that for every $j = 1, 2, \ldots, s$ $\|a_j - \tilde{a}_j\| + \|b_j - \tilde{b}_j\| < \epsilon_0$ and $\|v(a_j) - v(\tilde{a}_j)\| + \|v(b_j) - v(\tilde{b}_j)\| < \epsilon_1$ for some small $\epsilon_0, \epsilon_1 > 0$, where $v(a)$ denotes the velocity of the sample a. In the other words we join together the pairs of samples which has close spatial positions and close velocities. We then choose from the groups Γ_j m groups: $\Gamma_{j_1}, \Gamma_{j_2}, \ldots, \Gamma_{j_m}$ such that they have more than n_0 elements whereas the rest groups have less than n_0 elements for some $n_0 < n$. We call the pairs from the chosen m groups the selected pairs. The total number $\tilde{n}$ of all pairs a_j, b_j is now decreased comparatively with the total number n of pairs in the set B_0.

To reimburse the total number of pairs we add $n - \tilde{n}$ new pairs $(\tilde{a}, \tilde{b})$ to the selected pairs. This can be done differently; the canonic way to do it is called the cross-over. The cross-over procedure means that we generate the new pairs from the selected ones by the exchange of the samples between two arbitrary chosen pairs, e.g. we generate the pairs $\tilde{a}_2, \tilde{b}_1$ and $\tilde{a}_1, \tilde{b}_2$ from the pairs $\tilde{a}_1, \tilde{b}_1$ and $\tilde{a}_2 \tilde{b}_2$. Small discrepancy with the former total number n of the pairs can be overcome by the random choise of the pair we add to the joint ensemble.

We then repeat this procedure many times and obtain the sequence

$$B_0, B_1, \ldots$$

of the sets consisting of the pairs of samples corresponding to our two real particles: bullet and target. At the end of this sequence, determined by the time frame of considered process, we have the final set of the pairs of samples that bring us the approximation of the final quantum state.

We now show why this procedure of quantum state selection agrees with quantum mechanical description of two particle evolution. We have to show that the selected pairs bear the prevailing part of quantum probability for two real particles in comparison with the pairs excluded from the set B_0 in the first step. Indeed, for the selected k pairs the amplitudes they bear in sense of Feynman path integrals are close and the total probability to find the real pair (bullet, target) in the corresponding spatial position is about

$$|\sum_{j=1}^{k} \frac{1}{n}| = \frac{k}{n}, \tag{4.2}$$

die to the constructive interference of amplitudes, whereas for the not close (in the position and velocity) elements with the same total number k the probability to find the real pair (bullet, target) in the area corresponding to the positions of these k pairs will be about

$$|\sum_{j=1}^{k} \frac{\alpha_k}{n}| \approx \frac{\sqrt{k}}{n}, \tag{4.3}$$

that is much less than $\frac{k}{n}$ for large k. It follows from that the phases which are associated with the samples are distributed randomly for the pairs from the different groups. It means that the selection process works well if the number of all samples is large. Practically, it must be large enough to recognize the important features in the behavior of our real system, for example, the interference of the pair (bullet, target) as the whole through two slits, etc.

The main adventage of the selecting algorithm is that it requires only the initial set of samples, whereas if we describe the evolution along the way of Hilbert formalism, it needs the exponentially large amount of memory. The cost of this economy is that fast quantum algorithms are out of this way of simulation, as well as the quantum processes distributing the amplitude among too large space area without its valuable concentration. Quantum entangled states of types GHZ and W satisfiy this condition. This is why the selection of states of these two forms must be our first aim.

5. Numerical simulation of two-particle resonance scattering. H2+ molecular ion creation

5.1. The definition of the problem

Let's consider numerical simulation concerning with reaction of molecular ion creation in two particle scattering reaction. Both interacting particles are considered to be classical during almost all scattering process. In the simplest case one of these particles is Hydrogen atom and the other is proton.

One of the possible theories describing quantum transformations in two-particle collisions is Landau-Zener theory. These authors considered the problem of intersection and quasi-intersection of adiabatic terms of quasi-molecule, which consist of two atomic particles. They also considered quantum transitions during particles motion along these terms.

The term "quasi-molecule" means that the atomic particles are considered to be parts of the molecule independently on the distance between these particles. The description of that process in terms of quasi-molecules takes place when adiabatic approximation is correct.

5.2. Adiabatic levels, adiabatic (quasi-molecular) wave functions. Nonadiabatic operator

Adiabatic approximation takes place when velocities of nuclei are small enough (in comparison with electron's velocity), so that electron is considered to be in "motionless" nuclei environment (at any distance between nuclei). When this approximation comes true electronic and nuclei variables can be considered separately. Adiabatic energy levels which can be considered as function of the distance between atomic particles can be obtained as well. Nuclei motion is considered to be classical and is caused by potential, which equals to the sum of adiabatic energy and Coulomb interaction between nuclei.

Since adiabatic approximation has definite limit (the relative velocity of nuclei must be small enough, as it is described above, and large enough to consider nuclei motion classically), there are definite probability for quantum transition between adiabatic levels. These transitions are called nonadiabatic transitions. They are governed by nonadiabatic operator which in the typical case constitutes a derivation operator (by inter-particle distance).

To summarize the above, we can say that there is the basis of adiabatic (quasi-molecular) wave functions which corresponds to their eigenvalues - energies which depends on the distance of interacting particles.

5.3. Diabatic levels, diabatic (atomic) wave functions. Quasi-crossing of adiabatic terms

Adiabatic basis can be derived form so called diabatic states - i.e. pure atomic states. In our case diabatic states correspond to electron localization on first (or second) particle correspondently.

Let's consider two diabatic states which correspond to electron's state 1S (when electron is localized in the field of given particle). There is standard procedure for obtaining the matrix of the Hamiltonian and then diagonalizing that matrix.

$$\mathbf{H} = \left(\begin{array}{cc} H_{11} & H_{12} \\ H_{21} & H_{22} \end{array} \right) \tag{5.1}$$

Here H_{ij} is matrix element of two states Hamiltonian calculated between i and j diabatic states. H_{12} is considered to be constant - V.

After diagonalization of Hamiltonian we obtain the following:

$$\widetilde{\mathbf{H}} = \left(\begin{array}{cc} \widetilde{H_{11}} & 0 \\ 0 & \widetilde{H_{22}} \end{array} \right) \tag{5.2}$$

Here $\widetilde{H_{\alpha\beta}}$ is matrix element of two states Hamiltonian calculated between α and β adiabatic states. Diagonal elements of $\widetilde{H_{\alpha\beta}}$ represent correspondent adiabatic terms $E_I(R), E_{II}(R)$

$$\widetilde{H_{11}} = E_I = \frac{\widetilde{H_{11}} + \widetilde{H_{22}}}{2} + \sqrt{\frac{(\widetilde{H_{11}} - \widetilde{H_{22}})^2}{4 - V^2}} \tag{5.3}$$

$$\widetilde{H_{22}} = E_{II} = \frac{\widetilde{H_{11}} + \widetilde{H_{22}}}{2} + \sqrt{\frac{(\widetilde{H_{11}} - \widetilde{H_{22}})^2}{4 - V^2}} \tag{5.4}$$

Considering the region where diabatic terms cross we see that adiabatic terms avoid crossing. So we can say that adiabatic terms form quasi-crossing

According to von Neumann's theorem adiabatic terms of the same symmetry can't cross. Only the terms with different symmetry can cross. The region of quasi-crossing of adiabatic terms is the region of critical interest in Landau-Zener theory because quantum transitions take place when nuclei move along this region.

5.4. Landau-Zener theory for quasi-crossing adiabatic terms.

The two particle system can be investigated using Landau-Zener theory when it is possible to point out the isolated point of diabatic terms crossing. In that model the off-diagonal element of Hamiltonian matrix is considered to be constant. Particles move along the adiabatic terms up to the quasi-crossing region. The probability of nonadiabatic quantum transition is calculated in the quasi-classical limit by evaluation of integral of quasi-classical wave function's product. These wave functions correspond to initial and final adiabatic levels of nuclei in the quasi-crossing region.

$$P = \int e^{-i \int_0^\infty (E_I(R) - E_{II}(R)) dt} dR \tag{5.5}$$

The asymptotic exponential limit of quantum transition probability can be evaluated by considering the complex values of distance between particles. Thus adiabatic

terms can cross when imaginary part of distance is nonzero. Such crossing is essential feature of adiabatic term. Probability of quantum transitions in the above problem can be obtained by analysis of position of such crossing only.

5.5. Resonance quantum transitions during two particles scattering — the absence of quasi-crossing. Soloviev's model

Reactions (quantum transitions) during resonance and quasi-resonance scattering can not be considered using Landau-Zener model. This is impossible to point out the quasi-crossing region for the quasi-molecule in this case. Figure 1 indicates the essential features of adiabatic terms. Terms merge at large (infinite) distance, so quasi-crossing region is absent for reaction of this type.
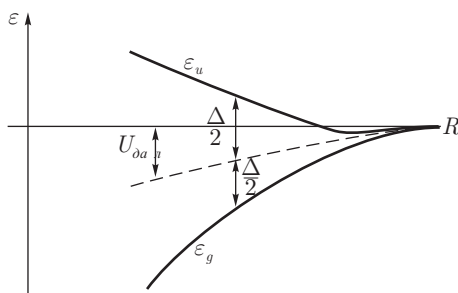

Fig. 1. Adiabatic terms for quasi-molecules which consists of 2 identical atomic particle and one valent s-electron.[15]

Here term ϵ_u corresponds to anti-symmetric combination of wave functions, ϵ_g corresponds to symmetric combination, Δ - exchange coupling. Electron wave functions of g and u state are stated below:

$$\Psi_g = (\psi_1 + \psi_2)/\sqrt{2} \qquad (5.6)$$

$$\Psi_u = (\psi_1 - \psi_2)/\sqrt{2} \qquad (5.7)$$

Here ψ_1 and ψ_2 are electron atomic wave functions which correspond to $1S$ electron state of first (or second) particle correspondently.

These wave functions are exact wave function of system considered in the adiabatic limit. Transitions between correspondent adiabatic terms take place due to exchange coupling only.

This is necessary to consider such system using theory described in **rev**. According to this theory there are two series of quasi-crossing in the case of resonance scattering (crossing when the distance between particles is considered having imaginary part). Using the rev terminology one of these series is called S-seria and the other is called T- seria. In the region corresponding to S-seria there are quasi-crossing of adiabatic terms with the different main quantum number and with the same quantum

numbers of angular moment and it's projection: $E_n lm(R)$ $_n + 1 lm(R)$ consequently for every $n >= l + 1$.

In the case of T-seria, quasi-crossings corresponding to terms with different quantum numbers of angular moment and its projection take place.

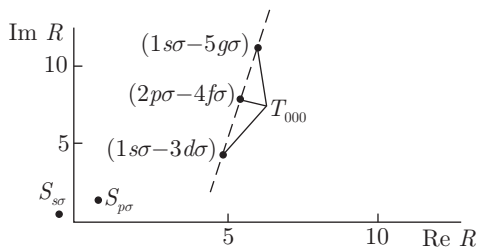Figure 2 depicts S-seria and T-seria. S-seria looks like dot because of scale discrepancy.

Fig. 2. S-seria and T-seria of quasi- adiabatic terms crossing for H_2+ molecular ion [14]

Physically this picture of electron behavior means that there are two characteristic lengths (which belong to different series of quasi-crossing) in considered system: R_s and R_t.

When inter-particle distance becomes equal to R_t, electronic wave function is changed dramatically. It corresponds to the process when electron (considered classically), which initially moved in the vicinity of one-well potential, becomes affected by double-well potential. Quantum mechanical transformations in this case correspond to initial angular moment distribution over all set of angular moments.

When inter-particle distance becomes equal to Rs, transitions with change of main quantum number take place. In connection with this the following "classical" analogy can be done: in that region the relaxation of electron energy over the total set of main quantum number take place.

Figure 3 depicts the electronic processes and correspondent spatial region.

The Figure 4 depicts the plots of adiabatic terms for molecular ion H_2+. The R_s region corresponds to sharp promotion of diabatic term to the continuous spectrum. These regions depend on angular momentum of electron.

5.6. Numerical simulation of reaction of molecular ion creation. Algorithm.

In the numerical simulation the resonance two particle scattering problem was investigated. One particle of interest was simplest atomic particle (nucleus plus electron) and another particle was positive ion (nucleus). There were two extra parameters in numerical experiments, which correspond to R_t and R_s from the above consideration.

We are interested in the integral characteristics of process:

1. (Reactions)/(Total experiments) ratio as function relative velocities.
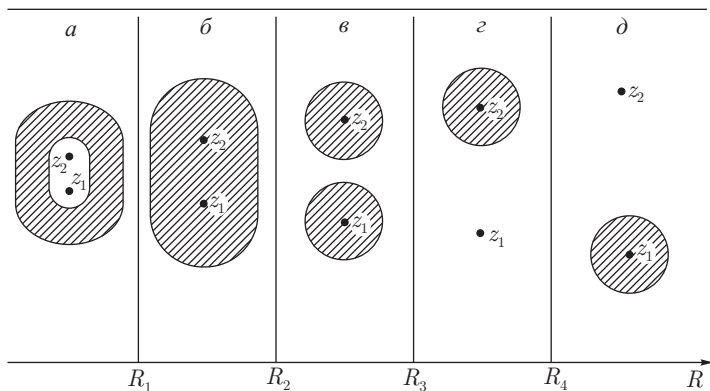
Fig. 3. The regions of electron motion classically permitted during molecular ion creation [14]
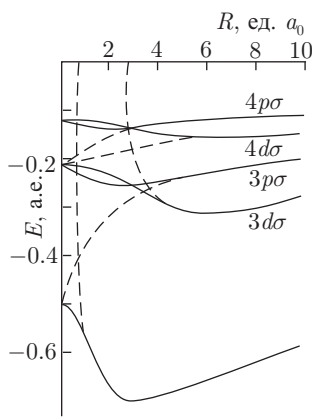
Fig. 4. Adiabatic terms (solid) and diabatic terms (dashed) for H_2+ molecular ion [16]

2. Reactions profile distribution.

3. Reactions threshold.

Below are listed the essential features of program algorithm used

1. The sets of numerical experiments were performed. Each set of experiment was configured separately. In each experiment, belonging to the given set, impact parameter slightly differed from one of previous experiment. Initial velocities were constant along all experiment set. Then the next set of experiments was executed with the other value of initial velocities. And so on.

2. Initially (when inter-particle distance R was greater then R_t) ($R > R_t$) potential of inter-particle interaction (i.e. adiabatic term) was considered to be equal U_1.

3. When moving particles initially becomes closer then Rt, but farther then R_s ($R_t < R < R_s$) potential was considered to be equal still U_1. Reaction did not take place.

4. When distance between particles becomes equal R_s potential was considered to be equal still U_2 — reaction occurred.

5. Particles moved under influence of potential U_2 — (i.e. particles performed molecular ion) until inter-particle distance becomes equal R_t again. After that potential becomes equal U_1 — (i.e. reaction of dissociation took place).

5.7. Results

The aim of experiments was to demonstrate quality behavior of two-particle resonance scattering influenced by quantum transitions. So all characteristic values used in experiments (i.e. potential constants, mass, lengths, velocities etc.) were not in correspondence with real world constants.

Potentials considered were the functions of inter-particle distance R only.

U_1 was chosen as standard ion — atomic potential in a long distance limit:

$$U_1 = -\frac{\alpha}{R^4} \tag{5.8}$$

U_2 — harmonic potential in a form:

$$U_2 = k(R - R_0)^2 + U_0 \tag{5.9}$$

Constants α, k, R_0, U_0, R_t, R_s were chosen 2.0, 10.0, 1.0, -5.0, 1.85, 1.8.

Every experiment in every set takes 5000 steps. Impact parameter step ρ_s was 0.04. In every experiments in the set impact parameter was incrementally increased by ρ_s from 0 (in initial experiment) up to $N_{exp} * \rho_s$ in final experiment. Here N_{exp} is number of total experiments in the given experiment set.

Constants N_{exp}, ρ_s were chosen 350 and 0.04 in every experiment set.

Initial inter-particle distance was chosen 15.0 in every set. Initial relative velocity was constant in every experiment set and consequently changed from one experiment set to the other.

Reaction profile means the following. During experiment execution there were the situations when particles were (e.g.) first associated (A), then dissociated (D), then once again associated (A). Such reaction is denoted as R_{ADA} or R_3. Correspondingly R_1 means R_A, R_2 means R_{AD}, R_4 means R_{ADAD}, R_5 means R_{ADADA} and so on.

Results of some experiment's set are stated in the below tables.

Table 1. Initial relative velocity is 0.5.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	220	176	36	8	0	0	8.76

Table 2. Initial relative velocity is 0.4.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	241	187	44	8	1	1	9.6

Table 3. Initial relative velocity is 0.375.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	247	201	35	10	1	0	9.84

Table 4. Initial relative velocity is 0.35.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	252	209	34	8	0	1	10.04

Table 5. Initial relative velocity is 0.25.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	266	214	43	8	1	0	10.06

Table 6. Initial relative velocity is 0.125.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	253	193	59	2	0	0	10.12

Table 7. Initial relative velocity is 0.05.

N_{exp}	TR	R_i					ρ_{tr}
		R_1	R_2	R_3	R_4	R_5	
350	224	187	37	0	0	0	8.92

In the above tables: N_{exp} — total experiments in the set, always equal 350.

TR — total reactions during set execution. This means that during experiment execution reaction happened more than one time.

R_i — total number of reaction of given profile.

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Quantum search algorithm for graph isomorphism problem

In this article I would like to present a quantum algorithm that solves graph isomorthism problem for two graphs with n vertices with complicity $O((n!)^{2/5} \cdot n^2)$. It is a slightly changed version of quantum search algorithm for element distinctness made by Andris Ambainis.

1. Introduction

This paper consists of 4 sections: Introduction, Ambainis algorithm overview, Algorithm for graph isomorphism and Conclusion. We will begin with definitions of our problems and some graph theory facts. In Introduction we will also discuss an element distinctness and compare it with graph isomorphism problem.

Main problem: *Let G_1, G_2 be two graphs. Check if they are isomorphic.*

Note: *Two graphs $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2)$ (V_1, V_2-sets of vertices, E_1, E_2-sets of edges) are called isomorphic if there exists one-to-one correspondence(we will call this correspondence "target correspondence") between thier sets of vertices, such that for each pair $v_{11}, v_{12} \in V_1$:*

$$(v_{11}, v_{12}) \in E_1 \Rightarrow (v_{21}, v_{22}) \in E_2 \text{ and } (v_{11}, v_{12}) \notin E_1 \Rightarrow (v_{21}, v_{22}) \notin E_2$$

where $v_{21}, v_{22} \in V_2$-vertices that correspond to v_{11}, v_{12} respectively.

By default, later in text, we will consider our graphs to have same number of vertices(if number of vertices differs then they aren't isomorphic) $|V_1| = |V_2| = n$. We will also consider that each of vertex sets V_1, V_2 has some default numeration of vertices: $V_1 = (v_{11}, v_{12}, ..., v_{1n}), V_2 = (v_{21}, v_{22}, ..., v_{2n})$ and edge sets E_1, E_2 contain pairs of vertex indexes not vertices.

Definition:(Graph renumeration) *Let $G_1 = (V_1, E_1)$ be a graph(with default numeration of vertices). $G_1^{(i_1,i_2,...,i_n)} = (V_1', E_1')$ where $v_{11}' = v_{1,i_1}$; $v_{12}' = v_{1,i_2}$; ...; $v_{1n}' = v_{1,i_n}$, $i_k \neq i_l$, $k \neq l$, $i_j \in \{1, 2, ..., n\}$, $j \in \{1, 2, ..., n\}$ is called $(i_1, i_2, ..., i_n)$-remuneration of graph G_1 (E_1 is converted to E_1' by changing indexes of vertices in pairs, for example: $(i_k, i_l) \rightarrow (k, l)$).*

Note: *Any renumeration of a graph G is isomorphic to G and any graph isomorphic to G is its renumeration becase all $n!$ possible graph renumerations covers all one-to-one vertex correspondances.*

We can say that searching for target correspondence for G_1, G_2 is the same as searching for renumerations $G_1^{(i_1,i_2,...,i_n)} = (V_1', E_1')$ and $G_2^{(j_1,j_2,...,j_n)} = (V_2', E_2')$ of

that graphs such that for each $v'_{1i}, v'_{1j} \in V'_1 : (v_{1i}, v_{1j}) \in (\notin)E'_1 \Rightarrow (v'_{2i}, v'_{2j}) \in (\notin)E'_2$,where $v'_{2i}, v'_{2j} \in V'_2$.

Definition:(Incidence matrix) *Let $G = (V, E)$ be a graph, $|V| = n$. Matrix $A_G = \{a_{ij}^G\} \in \{0,1\}^{n \times n}$, where $a_{ij}^G = 1 \Leftrightarrow (v_i, v_j) \in E$ is called the incidence matrix of G graph.*

Note: *If two graphs G_1, G_2 have same incidence matrixes, then they are isomorphic with target correspondence: $v_{11} \leftrightarrow v_{21}, v_{12} \leftrightarrow v_{22}, ..., v_{1n} \leftrightarrow v_{2n}$. As a result, if two graphs G_1, G_2 have renumerations $G_1^{(i_1, i_2, ..., i_n)}, G_2^{(j_1, j_2, ..., j_n)}$ with same incidence matrixes, then they are isomorphic with correspondence $v_{1,i_1} \leftrightarrow v_{2,j_1}, v_{1,i_2} \leftrightarrow v_{2,j_2}, ..., v_{1,i_n} \leftrightarrow v_{2,j_n}$.*

We can define any renumeration of given graph G with one parameter:an ordered set of different n indexes $\{1, ..., n\}$, so as we can code all such sets using numbers from 1 to $n!$ and each set will have an unique number, we can say that any graph renumeration have one parameter - natural number from $\{1, ..., n!\}$. Let's can define a matrix $A_G(l) \in \{0,1\}^{n \times n}, l \in \{1, ..., n!\}$ - that is an incidence matrix of lth-renumeration (renumeration with l parameter value) of graph G.

Now we are ready to define an oracle for our problem. At first we will define a base oracle, that will be used to make a more complex oracle for our algorithm. Base oracle is needed for easy comparison with other graph isomorphism algorithms.

Base oracle: *Suppose we have graph $G = (V, E)$ with incidence martix $A_G = \{a_{ij}^G\}$.*

$$f_G : |i, j\rangle \otimes |0\rangle \rightarrow |i, j\rangle \otimes |a_{ij}^G\rangle$$

f_G-*base oracle for graph G.*

Base oracle returns the smallest piece of information we can know about graph — for two indexes it checks if they are connected with an edge.

Algorithm oracle: *Suppose we have k graphs $G_1, G_2, ..., G_k$.*

$$F : |i, l\rangle \otimes |q\rangle \rightarrow |i, l\rangle \otimes \left| (q + \tilde{A}_{G_i}(l)) mod 2^{n^2} \right\rangle$$

where $i \in \{1, .., k\}, l \in \{1, ...n!\}$ and $\tilde{A}_{G_i}(l)$ is an incidence matrix of l-renumeration of graph G_i,that is written string by string in a line(so we have n^2 of 0 and 1 in answer register).

Note: *To call algorithm oracle once we need to call base oracle n^2 times.*

Using this oracle we can run a Grover search algorithm to solve isomorphism ploblem. We can do this by fixing incidence matrix of one of the graph and searching for same matrix among all $n!$ incidence matrixes of another graph. This gives us $O(\sqrt{n!})$ of agorithm oracle calls or $O(n^2 \cdot \sqrt{n!})$ base oracle calls. Grover algoprithm doesn't use additional information provided by the fact that objects it is searching for are graphs. It searches for one paricular object in $n!$ objets and doesn't care of their nature or features.

Let's define an element distinctness problem.We need this definition to see how we can apply the solution of this problem to isomorphism.

Element distinctness: *Suppose we have a numbers:*

$$x_1, x_2, ..., x_N \in \{1, ..., M\}$$

check if they are all distinct.

Now we can reveal the main idea of graph isomorphism algorithm. Let's take our $2 \cdot n!$ incidence matrixes and check, if they are all distinct, but with the condition, that we search for matches of matrixes of **different graphs**. If we find any, then graphs are isomorphic. Note, that if graphs are isomorphic, then we have at least $n!$ of matching matrix pairs. And it is enough to find only one pair to prove that graphs are isomorphic. This fact gives an opportunity to solve isomorphism problem faster than Grover algorithm do.

2. Ambainis algorithm overview

As we want to change agorithm for element distinctness we need to provide its short discription and main ideas.

2.1. Main idea

Suppose we have an element distinctness problem (see above). Let $r \in N$, $r >= 2$ be a parameter. Consider a graph with $C_N^r + C_N^{r+1}$ vertices. Each of C_N^r vertices contains set of r indexes from $\{1, ..., N\}$ and each of other C_N^{r+1} contains set of $r + 1$ indexes from $\{1, ..., N\}$. Different vertices contain different sets of indexes.

Two vertexes are connected with an edge only if one of them contain r indexes- $I_{v1} = \{i_1, i_2.., i_r\}$ and the other contain $r + 1$ indexes- $I_{v2} = \{j_1, j_2.., j_{r+1}\}$, and $|I_{v2} \backslash I_{v1}| = 1$.

Let's start in any edge of the graph. Our task is to find one of the vertices that contain indexes of equal munbers $(x_i, x_j : x_i = x_j, i \neq j)$. We will search graph moving only between vertexes that are connected with an edge. At first we check r (or $r + 1$) numbers those indexes are in the starting point. When we move, we need to check no more then one new number becase incidence vertex sets differs in one index. So if you can find target vertex by S steps then you can solve an element dis tinctness by $r + S$ steps.

2.2. Algorithm

Oracle for element distinctness:

$$f : |i, a\rangle \rightarrow |i, (a + x_i) \bmod M\rangle$$

where register i contains $\lceil \log N \rceil$ qubits and register a contains $\lceil \log M \rceil$ qubits.

This oracle is used in two situations in the algorithm:

1. $|i, 0\rangle \xrightarrow{f} |i, x_i\rangle$ — writing information

2. $|i, x_i\rangle \xrightarrow{unitary} |i, (-x_i) \bmod M\rangle \xrightarrow{f} |i, 0\rangle$ — errasing information

In his article Ambainis solves wider problem–element k-distinctness (searching for a cortage of indexes $i_1, i_2, ...i_k$ such that $x_{i_1} = x_{i_2} = ... = x_{i_k}$). But we will consider $k = 2$ and solving element distinctness only.

Let $x_1, x_2, ..., x_N \in \{1, 2, ..., M\}$. Consider we have a Hilbert space H, $|H| = $ $= C_N^r M^r (N - r)$(in fact Ambainis algorithm uses two Hilbert spaces but in our overview we will need only one of them, the other is used to run quantum walks, and we don't need to look through them to adapt an algorithm for our purposes). Basis states are $|S, l, \bar{x}\rangle$ where $S \subseteq \{1, 2, ..., N\}$, $|S| = r$-set of indices register, $l \in \{1, 2, ..., N\}$, $l \notin S$ — "edge" register (contain an index you have to query to move to other state — "vetrtex"), $\bar{x} \in \{1, 2, ..., M\}^r$ — contain querried information.

1. Generate the uniform superposition:

$$\frac{1}{\sqrt{C_N^r (N - r)}} \sum_{|S|=r, y \notin S} |S, y\rangle \otimes |0\rangle$$

2. Query all x_i for $i \in S$. This gives us:

$$\frac{1}{\sqrt{C_N^r (N - r)}} \sum_{|S|=r, y \notin S} |S, y\rangle \otimes |x_i\rangle$$

3. t_1(the exact number of seps needed we will evaluate below) times repeat:

   (a) Apply the conditional phase flip $(|S, y, x\rangle \rightarrow -|S, y, x\rangle)$ for S such that $x_{i_1} = x_{i_2}$ for distinct $i_1, i_2 \in S$.

   (b) t_2 times perform quantium walk[1].

4. Measure the final state. If S contains needed indexes then answer "'yes"' otherwise answer "'no"'.

2.3. t_1 evaluation

We can evaluate t_1 as $O(\frac{1}{\alpha})$ where $\alpha = \sqrt{\alpha'}$, α'-fraction of S such that there are $i_1, i_2 : \{i_1, i_2\} \subseteq S$ and $x_{i_1} = x_{i_2}$(Note that it is a fraction of S we are searching for e.g. **the fraction of basis states affected by conditional fase flip step of algorithm**).

$$\alpha' = \frac{C_{N-2}^{r-2}}{C_N^r} = \frac{\dfrac{(N-2)!}{(r-2)!(N-r)!}}{\dfrac{N!}{r!(N-r)!}} = \frac{r(r-1)}{N(N-1)} = O(\frac{r^2}{N^2})$$

$$\alpha = O(\frac{r}{N}); t_1 = O(\frac{N}{r})$$

---

[1]We won't look through quantium walks in this paper. The only thing we need to know about this step is that each step querries oracle twice and t_2 in our case depends only on parameter r(it is a Hilbert space H parameter) and is equal to $O(\sqrt{r})$

2.4. Overal result

Overal number of oracle querries is

$$O(\max_{2 \le r \le N} (r, t_1 \cdot t_2)) = O(\max_{2 \le r \le N} (r, \frac{N}{\sqrt{r}})) = O(N^{2/3})$$

where r is set $N^{2/3}$ to archieve the minimum possible number of querries.

For implementation of this algorithm we require $O(r(logN + logM))$ qubits.

3. Algorithm for graph isomorphism

In this section we will describe changes we need to apply to algorithm for element distinctness to solve graph isomorphism problem.

3.1. Main ideas

Suppose we have two graphs G_1, G_2. Check if they are isomorphic.

In Introduction we have described two oracles for graph isomorphism problem. One of them — base oracle — recieves an ordered pair of indexes and if this pair is in edge set of the graph outputs 1 otherwise output is 0. Base oracle is used to compare this algorithm with others. With this oracle we have built exact oracle we need in the algorithm. It recieves index of the graph and code of renumeration of graph and outputs an incidence matrix.

We can look at our problem this way:

1. We have set of numbers(incidence matrixes writen string by string) $x_1, x_2, ..., x_N$, where $N = 2 \cdot n!, x_1, x_2, ..., x_N \in \left\{1, ..., 2^{n^2}\right\}$(each of incidence matrixes require n^2 bits).

2. Check if there are $i, j : x_i = x_j, i \in \{1, 2, ..., N/2\}, j \in \{N/2 + 1, ..., N\}$

Problem is similar to element distinctness problem with $2n!$ elements except we need to bother that equal elements have different first indexes(first indexes represent indexes of a graph and they need to be distinct to prove isomorphism).

The only step in graph isomorphism algorithm that is responsible for "marking" base states, as base states on witch we want to increase amplitude, is conditional fase flip step $(3a)$.

If we change condition in conditional fase flip step we also need to reevaluate t_1 becase its evaluation depends on fraction of base states that satisfy fase flip step condition among all base states.

3.2. Algorithm

Oracle for the algorith we have described in introduction it had two input registers - one is graph index, the other is renumeration code, but we can treat both of input

registers as one input register. In case of two graphs this cumulative input register can receive $2 \cdot n!$ different values. For simplicity let's say that it can be $1, 2, ..., 2 \cdot n!$

Algorithm is same as in section 2.2(except $(3a)$ step is converted to $(3a')$ step) where $M = 2^{n^2}, N = 2 \cdot n!$, exept $(3a)$ step. t_2 remains the same becase Hilbert space H have the same structure (so $t_2 = O(\sqrt{r})$), t_1 changes, its reevaluation we will provide below.

$3a'$. Apply the conditional phase flip $(|S, y, x\rangle \rightarrow -|S, y, x\rangle)$ for S such that $x_{i_1} = x_{i_2}$ for distinct $i_1, i_2 \in S$ and one of indexes is in $\{1, ..., N/2\}$ and the other in $\{N/2 + 1, ..., N\}$.

As the first qubit of oracle input register is the graph index qubit (0 for one graph and 1 for another),if input is in $\{1, ..., N/2\}$ then oracle will return incidence matrix of the first graph otherwise it will return an incidence matrix of the second graph.

3.3. t_1 reevaluation

$t_1 = O(\frac{1}{\sqrt{\alpha'}})$, where α' is a fraction of basis states with S register such that $x_{i_1} = x_{i_2}$ for distinct $i_1, i_2 \in S$ and one of indexes is in $\{1, ..., N/2\}$ and the other in $\{N/2 + 1, ..., N\}$.

In our algorithm $x_i, i \in \{1, 2, ..., N\}$ - incidence matrixes of some renumeration of the graphs. Consider the right answer of the problem is "'yes"' and our graphs are isomorphic. This means that there are a pair of renumerations of theese graphs with same incidence matrixes. If we apply to both theese renumerations **any** non-trivial renumeration(we call renumeration trivial if we don't actualy change index of any vertex), we recieve another pair of renumerations of initial graphs with same incidence matrixes. So if the answer is "'yes"' then we have one pair of equal incidence matrixes of different graphs, and there are at least another $n! - 1$ distinct pairs of equal incidence matrixes of different graphs.

Overal number of basis states is C_N^r. If answer of the problem is "'no"', then we will recieve it anyway and t_1 doesn't play any role. If answer is "'yes"', then fraction of basis states that contain equal incidence matrixes of different graphs can be evaluated this way:

1. Let $r = (n!)^q$,where $0 < q < 1/2, q \in \text{Re}$

2. Fix and numerate r^2 pairs from $n!$ pairs of equal matrixes of different graphs.

3. Count fraction of basis states that contain first pair.

$$N_1 = \frac{C_{N-2}^{r-2}}{C_N^r} = \frac{\frac{(N-2)!}{(r-2)!(N-r)!}}{\frac{N!}{r!(N-r)!}} = \frac{r(r-1)}{N(N-1)} = O(\frac{r^2}{N^2}) = O((n!)^{2q-2})$$

4. Count fraction of basis states that contain second pair and don't contain any member of the first pair(this prevents us from counting some states twice). So two indexes are fixed in S register and two are denied to be in S.

$$N_2 = \frac{C_{N-4}^{r-2}}{C_N^r} = \frac{\frac{(N-4)!}{(r-2)!(N-r-2)!}}{\frac{N!}{r!(N-r)!}} = \frac{r(r-1)(N-r)(N-r-1)}{N(N-1)(N-2)(N-3)} = \quad (3.1)$$

$$= \frac{(n!)^q((n!)^q-1)(2 \cdot n! - (n!)^q)(2 \cdot n! - (n!)^q - 1)}{2 \cdot n!(2 \cdot n! - 1)(2 \cdot n! - 2)(2 \cdot n! - 3)} = \quad (3.2)$$

$$= \frac{O((n!)^{2q+2})}{O((n!)^4)} = O((n!)^{2q-2}) \quad (3.3)$$

5. ....

r^2+2. Count fraction of states that contain r^2-th pair and don't contain members of any previous pair. So two indexes are fixed in S register and $2 \cdot (r^2 - 1)$ are denied to be in S.

$$N_{r^2} = \frac{C_{N-2(r^2-1)}^{r-2}}{C_N^r} = \frac{\frac{(N-2(r^2-1))!}{(r-2)!(N-2(r^2-1)-r+2)!}}{\frac{N!}{r!(N-r)!}} \quad (3.4)$$

$$= \frac{r(r-1)\overbrace{(N-2(r^2-1))(N-2(r^2-1)-1)...(N-2(r^2-1)-r+3)}^{r-2}}{\underbrace{N(N-1)...(N-r+1)}_{r}} = (3.5)$$

$$= \frac{O((n!)^{2q+r-2})}{O((n!)^r)} = O((n!)^{2q-2}) \quad (3.6)$$

r^2+3. $\alpha' > N_1 + N_2 + ... + N_{r^2} = r^2 O((n!)^{2q-2}) = O((n!)^{4q-2})$

So $t_1 = O(\frac{1}{\sqrt{\alpha'}}) < O((n!)^{1-2q})$. If we set $t1 = O((n!)^{1-2q})$ we will archive the result with constant probability.

3.4. Complicity and memory

Overal complicity is $O(\max((n!)^q, (n!)^{1-2q} \cdot (n!)^{q/2}))$. If we set $q = 2/5$ then we archive the minimum of complicity.

Complicity in terms of base oracle is $O(n^2 \cdot (n!)^{2/5})$.

Memory required: $O((n!)^{2/5}(\log(n!) + \log(2^{n^2}))) = O(n^2 \cdot (n!)^{2/5})$ of qubits.

4. Conclusion

Our algorithm solves graph isomorphism problem faster then Grover algorithm do. At the same time it requires a lot of memory — exponential memory. It is a variant of quantium walk algorith and it is based on Ambainis's algorithm for element distinctness. At the end I would like to notice that this algorithm can work faster as we can count fraction of basis states more precisely. It is an open problem.

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