Simulation Of Certain Quantum Effects

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Abstract

The article presents a way to describe and determine some of the main quantum effects by means of semantic networks. Semantic networks are defined in the object-oriented simulation language UML2 SP. It has been shown that the representation of scientific models using semantic networks is as effective as mathematical descriptions.

Keywords: simulation, OOS, ABS, MAS, quantum effects, semantic network, ontologies, scientific models, UML2 SP

1 Introduction

In our work [1] it was proposed that semantic nets may be used to describe scientific models along with mathematical descriptions. In the work [2] we proposed a description of relativistic effects using a semantic net. In this paper, in particular, we proposed an one approach to describing quantum effects using semantic nets.

A number of scientists have developed the idea that algorithms can be used to describe physical phenomena. In greatest detail this idea is described in books by Stefan Wolfram [3, 4]. In these books, using graphs (networks) as a basis for representing nature and then deriving the laws of physics from algorithms using the graphs has been proposed. A similar point of view is stated in G. Hooft's book [5].

Our approach develops this idea further on the basis of an object-oriented paradigm. Instead of algorithms, we propose considering the exchange of messages between objects. Since objects are instances of classes, and links (communications) are instances of associations, the scientific model can be described as a frame semantic network, in particular it can be seen as an ontological description.

In our opinion, the description of physical models in a language other than the language of mathematics will contribute to a deeper understanding of physical laws. In addition, using machine inference algorithms on frame semantic networks, one can obtain rather curious statements regarding nature of physical phenomena. The solution of this problem is also of practical importance for the construction of conceptual models of ABS in the field of nanotechnology.

The choice of concepts for models of quantum effects is based on one or another interpretation of quantum mechanics. At present, there are at least eleven interpretations of quantum mechanics. In this paper, we propose a description of quantum effects based on the concept of "affordances" [6]. This interpretation of quantum mechanics was first advanced by Werner Heisenberg and then developed by Vladimir A. Fock. According to this interpretation, quantum reality includes both objects in the classical sense and objects that exist only in the form of possibility or probability. This view is supported by both physicists and philosophers. A fairly detailed exposition of this interpretation is given in book [7].

This work has the following structure and the following issues will be considered:

- the double-slit experiment;
- the Principle of Uncertainty;
- quantum entanglement;
- Bell's test.

For each topic, a specific mathematical formulation is first given. Then a description in the language of semantic networks is given. After that, the results of the simulation experiment are presented, which are compared with the mathematical description.

In conclusion, we will summarize the work and in addition, a brief description of the repository that contains the simulation software will be given.

2 Key Points

To describe scientific models, we will use the language of object-oriented simulation UML2 SP [1]. This language is a profile of UML and is an object-oriented version of the well-known IDEF0 (SADT) methodology. The semantic network is built from frames, which are the "class" UML-element. Each frame is tagged "Concept". This tagged value is assigned a specific concept, which allows the building of a conceptual model of the problem domain.

Following the tradition of programming languages such as the Smalltalk and Python, we will treat both the classes themselves and class instances as objects. Class instances will be interpreted as objects of reality in the classical sense, and classes will be interpreted as objects that exist in possibility. Classes can also create new objects-class, so there won't be an endless chain of metaclasses.

Quantum effects may be described as follows.

1. Wave function analog is a class (in terms of computer science).

2. A wave function collapse analog is to run the constructor of the class and create an instance of the class. In addition, we separate the constructor call and the message for the measurement.

3. A quantum superposition analog is multiple inheritance. If the classes have attributes or operations with an identical name then multiple inheritance have a conflict of names. In this conflict, we will resolve the "quantum rule", i.e. using an amplitude of wave function. We note right away that complex numbers can be eliminated by replacing them with objects constructions, we will touch on this issue in the conclusion.

This will allow us to show how, based on these provisions, the main quantum effects can be described.

3 Double-Slit Experiment

3.1 Mathematical Description

Superposition cannot be observed directly, but the consequences of superposition can be observed. For example, in the double-path experiment, one can observe the interference of particles [8, p. 1-8].

Let x_0 be a particle source and x_1 be a point on screen. A particle can walk into x_1 in two paths. Denote by first path as a and second path as b. Then a wave function has view

$$|\psi\rangle = A_a|a\rangle + A_b|b\rangle,$$

here $A_a = c_a e^{i\varphi_a}$, $A_b = c_b e^{i\varphi_b}$ are complex numbers and c_a, c_b are real numbers.

Further, we find the coefficients c_a, c_b. We choose a normalization $|\psi\rangle$ so that

$$\int_0^{2\pi} \langle\psi|\psi\rangle d\varphi = 1,$$

and open the square of the amplitude

$$f(\varphi) = \langle\psi|\psi\rangle =| A_a |^2 + | A_b |^2 + (A_a^* A_b + A_a A_b^*) = c_a^2 + c_b^2 + 2c_a c_b \cos\varphi, \quad (1)$$

where $\varphi = \varphi_a - \varphi_b$. Then

$$2\pi c_a^2 + 2\pi c_b^2 + 2c_a c_b[\sin(2\pi) - \sin(0)] = 2\pi(c_a^2 + c_b^2) = 1.$$

If $c_a = c_b = c$ then

$$c = \pm\frac{1}{2\sqrt{\pi}}.$$

Formula (1) determines the interference pattern.

3.2 Semantic Net Description

The ontology of the double-slit experiment is depicted in Fig.1

The ontology is a similar ontology to the classical case but has a **Mix** class. The class inhered **move_to_x1** operation from both **A** and **B** classes. In this case, we have a conflict of names. This conflict resolves as the quantum rule. The **Mix** class has **z1** and **z2** attributes for the quantum rule. The **Composite** frame defines the abstract "Double-path experiment" concept. The **Node** frame defines a concrete experiment and determines the design of the experimental device.

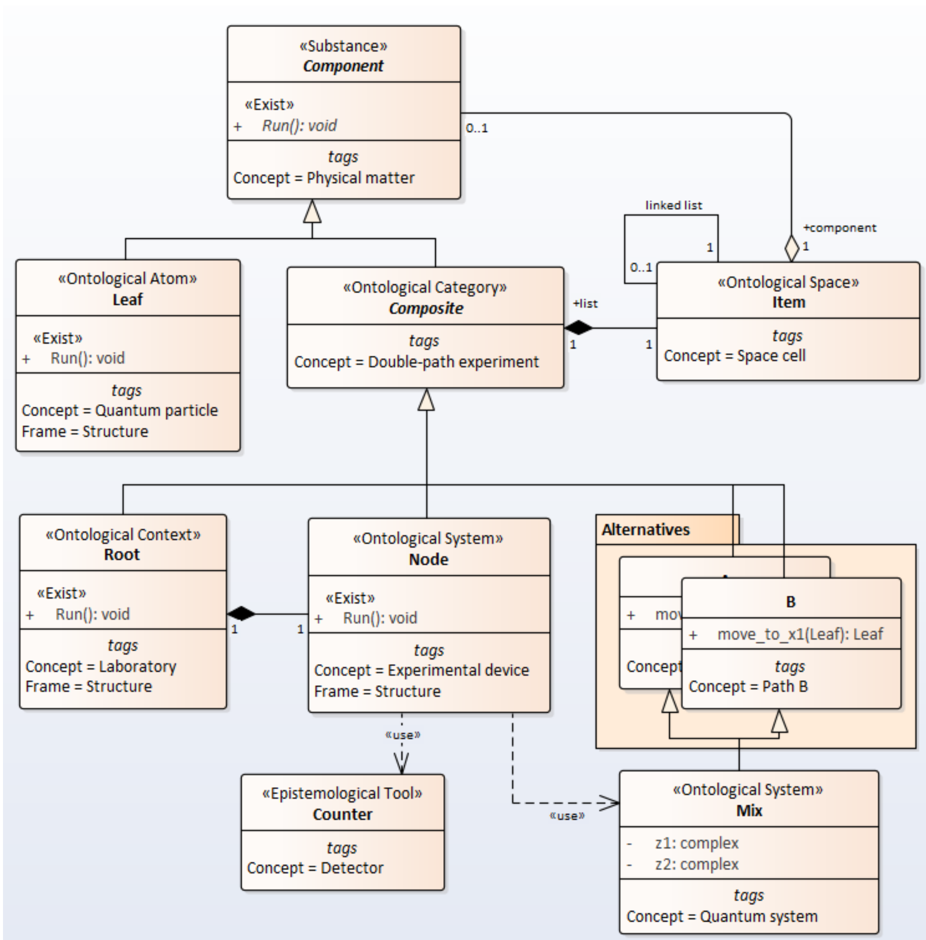

Figure 1: The ontology of the double-slit experiment

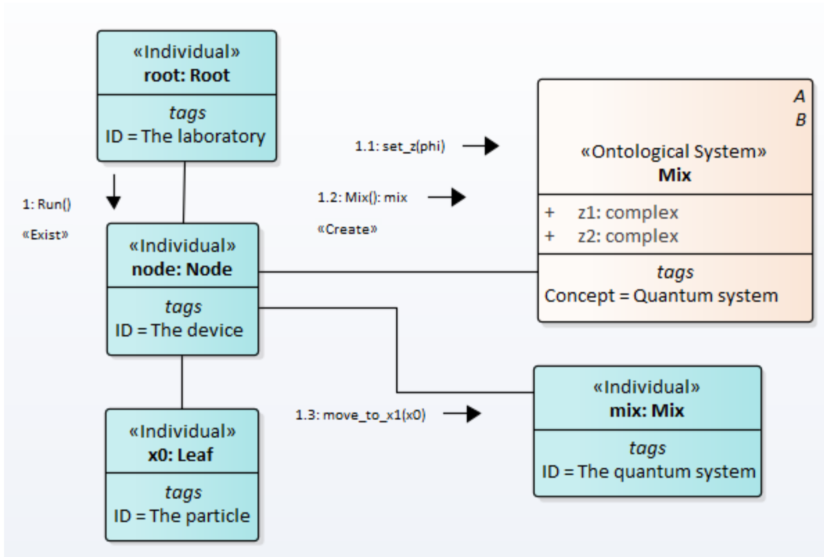

Figure 2: Single experiment

One step of the experiment is depicted in Fig.2.

The particle created and put to **x0** point. The **node** (experimental device) sends **set_z(phi)** message to the **Mix** class which sets both the **z1** and **z2** attributes. Further, the **node** creates an **a** object, where the names conflict is resolved. The next step is to execute the **move_to_x1(x0)** operation that places the particle at the **x1** point on the screen. This process executes a **Run()** operation many times in order to get the statistics. We observe that here, there is an elements of metaprogramming (Fig.2).

A typical result of the simulation experiment is depicted in Fig.3 (10 measurements for each value φ).

Note that if there are two different points **x1** and **x2** (operations **move_to_x1(x0)** and **move_to_x2(x0)**) then we get the classical case.

4 Uncertainty Principle

4.1 Mathematical Description

Consider the uncertainty principle [8, p. 1-17]. Let $\hat{L}$ and $\hat{M}$ be self-adjoint operators and their commutator $[\hat{L}, \hat{M}] = \hat{L}\hat{M} - \hat{M}\hat{L}$ be non-zero. Denote

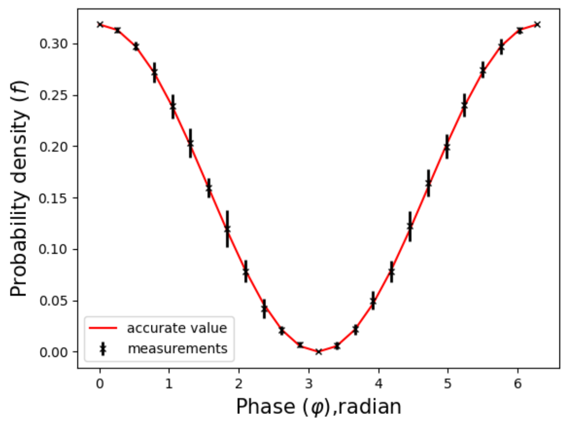

Figure 3: Interference pattern according to the results of the experiment

by $\mid l_i\rangle$ and $\mid m_j\rangle$, $i, j = 1, 2$ the eigenfunctions of these operators.

The wave function $\mid a\rangle$ can be written in the l-basis

$$\mid a\rangle = a_1 \mid l_1\rangle + a_2 \mid l_2\rangle$$

or in m-basis

$$\mid a\rangle = b_1 \mid m_1\rangle + b_2 \mid m_2\rangle$$

and

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} \langle m_1 \mid l_1\rangle & \langle m_1 \mid l_2\rangle \\ \langle m_2 \mid l_1\rangle & \langle m_2 \mid l_2\rangle \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}. \tag{2}$$

Denote a transformation matrix in (2) as U. The matrix U is a unitary matrix [9, p. 281]. By definition of a unitary operator, $|\det(U)| = 1$ and $U^{-1} = U^\dagger$ (because $\langle l_1 \mid m_2\rangle^* = \langle m_2 \mid l_1\rangle, \langle l_2 \mid m_1\rangle^* = \langle m_1 \mid l_2\rangle$).

Thus, we have five restrictions on the elements of the transformation matrix. The general expression of a 2×2 unitary matrix is

$$U = e^{i\varphi/2} \begin{bmatrix} e^{i\varphi_1} \cos\theta & e^{i\varphi_2} \sin\theta \\ -e^{-i\varphi_2} \sin\theta & e^{-i\varphi_1} \cos\theta \end{bmatrix}$$

For definiteness, let's choose, for example, this option: $\varphi = \varphi_1 = \varphi_2 = 0$, and $\theta = \pi/4$. Then the transformation matrix will look like

$$U = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$$

Accordingly, the elements of the matrix will take on the value $\langle m_1 \mid l_1 \rangle = 1/\sqrt{2}, \langle m_1 \mid l_2 \rangle = 1/\sqrt{2}, \langle m_2 \mid l_1 \rangle = -1/\sqrt{2}$, and $\langle m_2 \mid l_2 \rangle = 1/\sqrt{2}$.

Then we get uncertainty principle. Let be $a_1 = 1, a_2 = 0$. We get $b_1 = 1/\sqrt{2}$ and $b_2 = 1/\sqrt{2}$ from (2) . Let be $a_1 = 1/\sqrt{2}, a_2 = 1/\sqrt{2}$ then we get $b_1 = 1$ and $b_2 = 0$.

As we can see, if the measurement of one quantity is accurate then the other quantity is completely uncertain.

4.2 Semantic Net Description

The wave function as a semantic net is depicted in the Fig. 4.

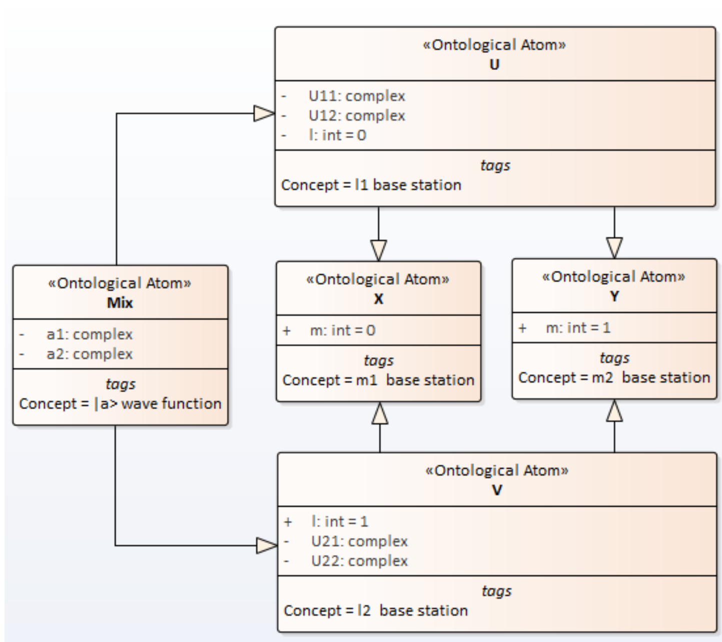

Figure 4: Describing the Uncertainty Principle using the semantic net

The names conflict (**l** and **m** attributes) is resolved twice. First in the constructor of the **U** and **V** classes, then in the constructor of the **MIX** class.

Table 1: The experimental frequencies of states

N	$\mid m_1\rangle$	$\mid m_2\rangle$	$\mid l_1\rangle$	$\mid l_2\rangle$
1	1.0	0.0	0.49 ($\pm$0.16)	0.51 ($\pm$0.16)
2	0.0	1.0	0.44 ($\pm$0.07)	0.56 ($\pm$0.07)
3	0.59 ($\pm$0.1)	0.41 ($\pm$0.1)	1.0	0.0
4	0.52 ($\pm$0.11)	0.48 ($\pm$0.11)	0.0	1.0

The simulation experiment result is represented in the table 1 (10 measurements).

As we can see, the uncertainty principle for these two limiting cases is satisfied.

5 Quantum Entanglement

5.1 Mathematical Description

In this section, we will look at quantum entanglement [9, p. 578]. Let a pair of particles be created at the S point. Particles fly in opposite directions. One of the particles enters detector A, the other - into detector B. We will not consider the EPR paradox, so we will consider quantum entanglement for only one property.

Let a quantum system be having two distinguishable particles. Each particle can be in two states: 0 and 1. In general, the wave function has the following form

$$|\psi\rangle = c_{00}|00\rangle + c_{01}|01\rangle + c_{10}|10\rangle + c_{11}|11\rangle.$$

If the particles are independent then the wave function has the form

$$|\psi\rangle = (c_0^1|0\rangle + c_1^1|1\rangle)(c_0^2|0\rangle + c_1^2|1\rangle),$$

and $c_{ij} = c_i^1 c_j^2, |ij\rangle = |i\rangle|j\rangle$, where $c_i^1, c_j^2, i, j = 0, 1$ are probability amplitude of the free particles.

If the system is in an entangled state then its wave function is

$$|\psi\rangle = c_{00}|00\rangle + c_{11}|11\rangle$$

or

$$|\psi\rangle = c_{01}|01\rangle + c_{10}|10\rangle$$

and the probability amplitudes are not equal to zero.

5.2 Semantic Net Description

Wave function as a semantic net is depicted in Fig.5. All classes **Two00**, **Two01**, **Two10**, **Two11** inherit the space with particles in the extreme cells. In the constructor of the **Mix** class, one of the alternatives is selected according to the square of the amplitude.

In code, the dependencies (**use** stereotype) are implemented as a global variable. This global variable first stores a pointer to the **Mix** class, then a pointer to an instance of the **Mix** class. This makes it possible to detect the particles both in the **SubnodeA** class and the **SubnodeB** class. We emphasize that we cannot use an operation call for this purpose, since the message must move through the **list** structure. This is the model of quantum nonlocality.

The message exchange order will be as follows, see Fig.6. As soon as **Alice** takes a measurement for the first particle, **Bob** can immediately find the state of the second particle, regardless of the distance between particles. This is possible because an instance of the **Mix** class already exists.

6 Bell's Test

6.1 Mathematical Description

In this section, we'll look at the Bell test [9, p. 582]. We will consider an analogue of the Stern-Gerlach experiment.

Stern-Gerlach devices L and R are located along the X axis and can rotate around this axis. Let +1 and -1 be a result of measurement, these are analogues of the projection of the spin "up" and "down".

Consider now Bell's theorem in form [10]. Denote by A, B, C three directions along which we will orient devices L and R. We will set these

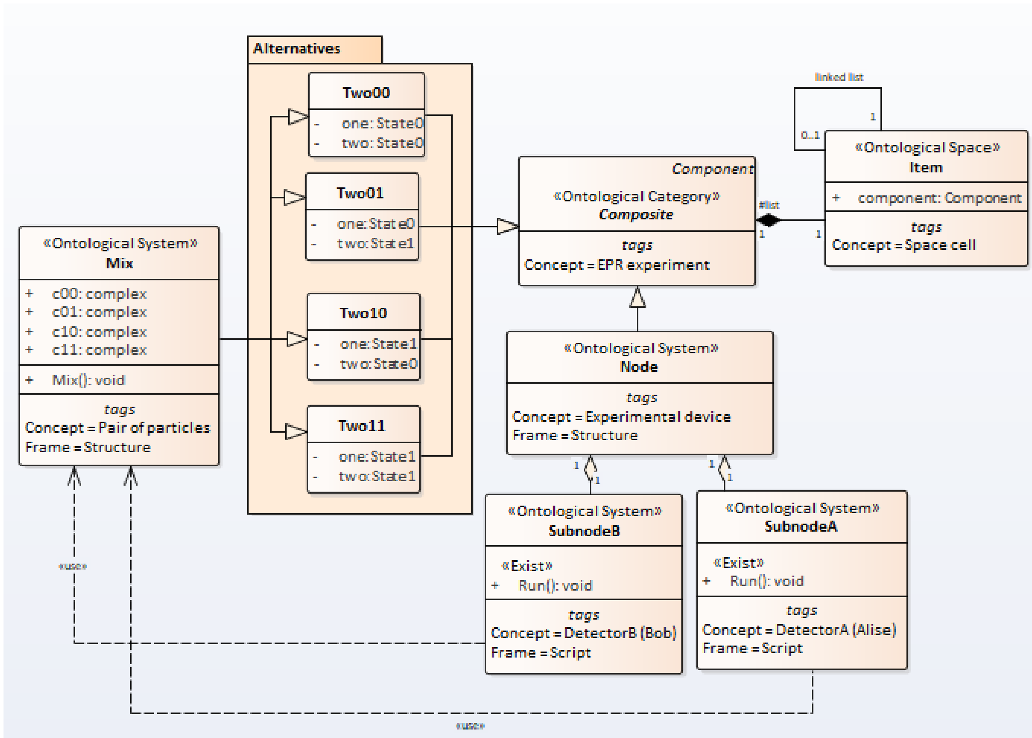

Figure 5: The pair of entangled particles model

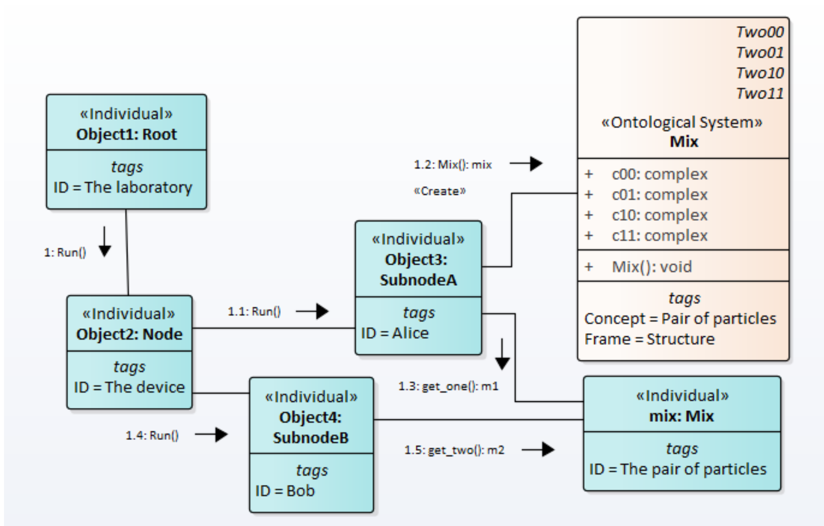

Figure 6: Sequence of messages in the EPR-experiment

directions for L and R in a completely random way. Let detector L give a result of +1 and detector R give a result of +1. The number of such pairs observed can be represented by the notation $n[A^+B^+]$.

Bell's inequality has the form

$$\frac{n[A^+B^+]}{n} \leq \frac{n[B^+C^+]}{n} + \frac{n[A^+C^+]}{n}, \tag{3}$$

here $n[...]/n$ is the frequency of the corresponding configuration, n - total number of measurements. From the point of view of the theory of hidden variables, this inequality must be satisfied for any of the directions A, B, and C.

From the point of view of quantum mechanics, we have an other result, denoted by P_{agree}, $P_{disagree}$ probabilities of coincidence and a mismatch. The formulas for these probabilities is [9, p. 587]

$$\begin{aligned} P_{agree} &= \frac{1}{2}(1 - \cos\alpha) = \sin^2(\frac{\alpha}{2}) \\ P_{disagree} &= \frac{1}{2}(1 + \cos\alpha) = \cos^2(\frac{\alpha}{2}), \end{aligned} \tag{4}$$

where α is the angle between the directions of the turn of devices L and R.

Let AB, AC, and BC denote the angle between directions A, B, C. The probability of an outcome is determined by the product of three probabilities: the probability that the experimental setup is in a given configuration (1/9), the probability that the measurement will give +1 or -1 (1/2), the probability of coincidence in the results of L and R. Then

$$\frac{n[A^+B^+]}{n} \approx P[A^+B^+] = \frac{1}{18}\sin^2(\frac{AB}{2}).$$

For AC, BC we obtain similar expressions, and inequality (12) takes the form

$$\sin^2(\frac{AB}{2}) \leq \sin^2(\frac{BC}{2}) + \sin^2(\frac{AC}{2}). \tag{5}$$

There are such mutual orientations of the directions A, B, C for which this inequality does not hold true.

6.2 Semantic Net Description

Let's check the formula first (4). We will use the same model as in section 5, only now we will rotate the device R around the X axis at different angles α. The dependence of the probability density on the angle of rotation is shown in Fig. 7 (10 measurements for each value α). We see that the simulation results fit well with the analytical curve (4).

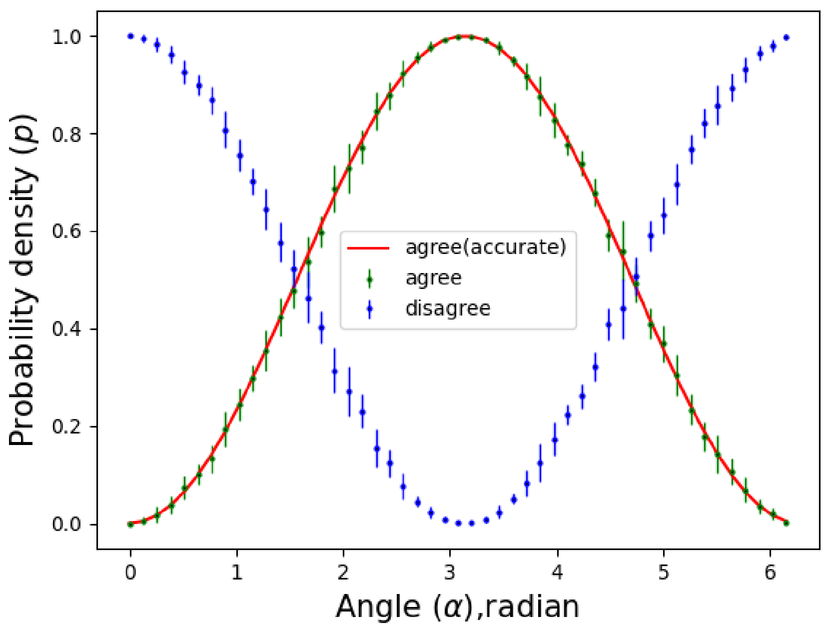

Figure 7: The probability density of the angle

Now let's run a simulation for Bell's test. We will use the same model as in section 5, only now the angle will take three values AB, BC, AC randomly. In simulated experiment, we measured the number of events and check the inequality

$$n[A^+B^+] \leq n[B^+C^+] + n[A^+C^+].$$

Some experiment results are depicted in table 2 (10 measurements for each combination AB, BC, AC).

Table 2: Results of testing Bell's inequality

№	AB	BC	AC	$n[A^+B^+]$	$n[B^+C^+]+n[A^+C^+]$	Result
1	315°	225°	50°	29(-0.98)	161(+2.58)	fulfilled
2	225°	45°	315°	144(-2.41)	52(+1.34)	not fulfilled
3	45°	135°	178°	20(-0.89)	308(+3.21)	fulfilled
4	90°	315°	48°	80(-1.78)	56(+2.9)	not fulfilled

We see that for the orientations of the second and fourth rows of the table, Bell's inequality does not hold. The results obtained correspond to expression (5). Other such combinations can be found.

Thus, the model in section 5 describes the quantum case.

7 Conclusions

Based on the above fragments of the semantic network, it is possible to construct an ontology of the considered quantum effects. The ontology has the same structure as in the classical case, except that the **Alternatives** package and the **Mix** class appear, as in Fig. 1. However, the construction of the ontology is hampered by several unresolved issues. In particular, the question of space and time in the microcosm is not clear. As mentioned above, metaprogramming must be used in the models. Therefore, a container for classes is needed. This is necessary for manipulating with class-objects. This raises the question of space modeling for class-objects. In the models considered, the physical space is structured only for classical objects. The question of space and time in the quantum world requires a separate study.

The transition from the quantum model to the classical one occurs if the name conflict is eliminated in the model. As a rule, in such cases it is possible to avoid multiple inheritance. In classical and relativistic mechanics, models are also described in the form of a class diagram. This means that semantic-network models initially have a common descriptive basis for both classical and quantum descriptions.

Note that another way of describing quantum effects is possible. This alternative approach is based on the "Decorator" design pattern (by GoF). We associate this approach with the formalysm a "path integral" by R. Feynman.

We plan to explore this issue in subsequent publications.

The software for this article is presented on the repositry [11]. The software is implemented in Python 3. An extended description of the quantum effects described above is given, documentation for the software is presented, and experimental results are presented. The resource also discusses some additional issues of quantum theory.

An ontology for the Reseford scattering for the quantum and classical cases is considered. Both ontologies are compared. It is shown how the transition from the quantum case to the classical case occurs.

The definition of spin by means of semantic networks is given. For this purpose, an analogue of the fibred space for spin 1/2 is used.

In our opinion, the main drawback of the proposed approach is that complex numbers are used to resolve the name conflict. We are not ready to accept the ontological character of complex numbers. In addition, this prevents the detailing of the model, since numerical simulation has to be used.

A non-numerical model is proposed and considered. An ordered pair of looped lists is used to eliminate complex numbers. The main processes with this data structure are defined. Based on this construction, a Hilbert's space model is constructed. A model for the collapse of the wave function is proposed. The processes that are described by the time-independent and time-dependent Schrödinger equations are considered.The problem of space and time in quantum mechanics is considered.

This model gives an idea of what a more detailed quantum mechanics model might look like. We do not present this model in this paper, since the model requires additional hypotheses about the quantum world. But the description of this model can be found in the repository.

The repository will be updated with new materials.

References

[1] Gurianov V.I.: A Brief Overview of the UML Scientific Profile, arXiv:2104.10042 (cs.DC), arXiv [Internet]. 2021. Available from: https://doi.org/10.48550/arXiv.2104.10042

[2] Gurianov V.I.: Simulation model of spacetime with the Minkowski met-

ric. arXiv:2009.10689 [cs.CE], arXiv [Internet]. 2020. Available from: https://doi.org/10.48550/arXiv.2009.10689

[3] Wolfram S.: A New Kind of Science, free E-Book, 2002, Available from: https://www.wolframscience.com/nks/

[4] Wolfram S.: A Class of Models with the Potential to Represent Fundamental Physics, arXiv:2004.08210, 2020, Available from: https://doi.org/10.48550/arXiv.2004.08210

[5] Hooft G.: The Cellular Automaton Interpretation of Quantum Mechanics, arXiv:1405.1548, 2015, Available from: https://doi.org/10.48550/arXiv.1405.1548

[6] Harre R.: Intern.Studies in the Phil. of Science, V.4,2,1990.

[7] Sevalnikov A.Y.: Interpretations of quantum mechanics: In search of a new ontology. M.: Book house "LIBROKOM", 2009.

[8] Feynman R, Leighton R, and Sands M. The Feynman Lectures on Physics, Volume 3: Quantum mechanics. NEW MILLENNIUM EDITION

[9] Penrose R.: The Road to Reality: A Complete Guide to the Laws of the Universe, Jonathan Cape, 2004

[10] D'Espagnat B. (1979): The Quantum Theory and Reality, Scientific American: 241 (5): 158–181, Available from: http://www.sciam.com/media/pdf/197911_0158.pdf

[11] Gurianov V.I.: Ontologies in Quantum Mechanics, GitHub repository, GitHub, 2023, Available from: https://github.com/vgurianov/qm